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NEWS 24 JAN 29 PHAR reloaded with new search and display fields NEWS 25 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases NEWS 26 FEB 13 CASREACT coverage to be extended NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records
NEWS 25 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases NEWS 26 FEB 13 CASREACT coverage to be extended NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records
multiple databases NEWS 26 FEB 13 CASREACT coverage to be extended NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records
NEWS 26 FEB 13 CASREACT coverage to be extended NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records
NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records
NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
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10/560,013 02/26/2007 .

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chain nodes :
16  17
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13
chain bonds :
13-16  16-17
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  7-10  8-9  8-13  10-11  11-12  12-13
exact/norm bonds :
5-7  6-9  7-8  7-10  8-9  8-13  10-11  11-12  12-13  13-16  16-17
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
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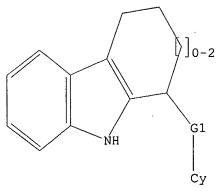
G1:NH,O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 16:CLASS 17:Atom

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS



G1 NH,O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 12:28:47 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -809229 TO ITERATE

100.0% PROCESSED 809229 ITERATIONS (3 INCOMPLETE) SEARCH TIME: 00.00.07

253 ANSWERS

253 SEA SSS FUL L1

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=> s 12 L3 ·

L3 · 33 L2

=> d ibib abs hitstr 1-33

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L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1207231 CAPLUS
DOCUMENT NUMBER: 145:489914

TITLE: Preparation of carbazoles and related compounds for treatment of dengue fever, yellow fever, west nile virus, and hepatitis C virus infection.

Gudumudasson, Kristjan
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
PCT Int. Appl. . 59pp.
CODEN: PIXXD2

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2006:121467 A2 20061116 W0 2005-US41091 20051114

WO 2006:121467 A2 20061116 W0 2005-US41091 20051114

WO 2006:121467 A3 20070125

W: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CK, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EZ, EG, ES, FI, GB, GD, GE, GH, GH, HR, HU, ID, II, IN, IS, JF, KE, KG, MM, KM, KF, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LV, LY, MA, MD, MG, MK, MM, MM, MX, AM, NG, NI, NO, NZ, OM, PG, PH, PP, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RN: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, LE, LS, MM, MX, NX, NM, NX, NM,
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L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ttion due to flaviviruses, pestiviruses, and hepaciviruses. Thus, 6-chloro-N-phenyl-2,3,4,9-tetrahydro-1H-carbazol-1-amine (preparation

outlined)

RN 812649-16-4 CAPLUS
CN 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)(9C1) (CA INDEX NAME)

RN 812649-17-5 CAPLUS
CN 1H-Carbazol-1-amine, 6-chloro-N-(4-chlorophenyl)-2,3,4,9-tetrahydro(9C1)
(CA INDEX NAME)

RN 812649-18-6 CAPLUS
CN 1H-Carbazol-1-amine, 6-chloro-N-(4-fluorophenyl)-2,3,4,9-tetrahydro(9CI)
(CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) showed anti-HCV activity with IC50 = 5 nM.

IT 812649-13-1P 812649-14-2P 812649-15-3P 812649-16-P 812649-16-P 812649-13-P 812649-17-5P 812649-18-PP 812649-21-1P 812649-22-P 812649-23-3P 812649-21-1P 812649-22-P 812649-23-3P 812649-22-PP 812649-27-PP 812649-27-PP 812649-28-PP 812649-29-9P 812649-30-2P 812649-31-3P 812649-31-7P 812649-31-3P 812649-31-3P 812649-31-3P 812649-31-3P 812649-31-7P 812649-31-3P 8126

● HC1

RN 812649-15-3 CAPLUS CN 1H-Carbazol-1-amine, 6-chloro-2, 3, 4, 9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-19-7 CAPLUS
CN 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methylphenyl)(9CI)
(CA INDEX NAME)

RN 812649-20-0 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)(9CI)
(CA INDEX NAME)

RN 812649-21-1 CAPLUS

L3 - ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Carbazol-1-amine, 6-bromo-N-(4-chlorophenyl)-2,3,4,9-tetrahydro-(CA INDEX NAME)

812649-22-2 CAPLUS 1H-Carbazol-1-mdine, 6-bromo-N-(4-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-23-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyrimidinyl-,monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

812649-27-7 CAPLUS
1H-CArbazol-1-amine, 6-chloro-N-(4,6-dimethyl-2-pyrimidinyl)-2,3,4,9-tetrahydro-(SCI) (CA INDEX NAME)

812649-28-8 CAPLUS
1H-Carbazol-l-amine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyridinyl-,monohydrochloride (9CI) (CA INDEX NAME)

• HCl

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HC1

812649-24-4 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

812649-25-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4,6-dimethoxy-2-pyrimidinyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-26-6 CAPLUS

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (9CI) (CA INDEX NAME) (Continued)

812649-30-2 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyrimidinyl- (9CI)
(CA INDEX NAME)

812649-31-3 CAPLUS 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methoxy-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 812649-32-4 CAPLUS CN 1H-Carbazol-1-amine, N-(4,6-dimethoxy-2-pyrimidinyl)-2,3,4,9-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HC

RN 812649-33-5 CAPLUS
CN IH-Carbacol-l-amine, 6-bromo-N-(4,6-dimethyl-2-pyrimidinyl)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

• HCl

RN 812649-34-6 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[5-{trifluoromethyl}-2-pyrimidinyl}- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-37-9 CAPLUS
CN 1H-Carbazol-1-amine, N-2-benzothiazolyl-6-bromo-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

RN 812649-38-0 CAPLUS (NAME) 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 812649-39-1 CAPLUS CN Cyclohept[b]indol-6-amine, 2-bromo-5,6,7,8,9,10-hexahydro-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

RN 812649-41-5 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyridinyl-,
monohydrochloride (SCI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-35-7 CAPLUS
CN lH-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-{5-(trifluoromethyl}-2-pyridinyl]- (SCI) (CA INDEX NAME)

RN 812649-36-8 CAPLUS
CN 3-Pyridinecarbonitrile, 6-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-y1)amino]- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HC1

RN 812649-42-6 CAPLUS
CN 1H-Carbazole-6-carboxylic acid, 2,3,4,9-tetrahydro-1-(phenylamino)-,
methyl ester (9C1) (CA INDEX NAME)

RN 812649-44-8 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 812649-45-9 CAPLUS CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

NHPh H

RN 812649-46-0 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(3-methoxyphenyl)-(9CI) (CA INDEX NAME)

MeO NH H N

RN 812649-47-1 CAPLUS CN 1H-Carbacol-1-amine, 6-bromo-N-(3-fluorophenyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

F NH H

RN 812649-48-2 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-1H-indol-5-yl- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

F NH

RN 812649-52-8 CAPLUS
CN 1H-Carbazol-l-amine, 6-bromo-N-(3,4-dichlorophenyl)-2,3,4,9-tetrahydro(9C1) (CA INDEX NAME)

C1 NH H H

RN 812649-53-9 CAPLUS
CN 1H-Carbazole, 6-bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 814255-17-9 CAPLUS
CN 3-Pyridinecarbonitrile, 6-[(2,3,4,9-tetrahydro-6-methyl-1H-carbazol-1yl)amino|- [9:1] (CA INDEX NAME)

L3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

RN 812649-49-3 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(2-methoxyphenyl)(9CI)
(CA INDEX NAME)

Meo NH H

RN 812649-50-6 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(2-chlorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

c1 NH H

RN 812649-51-7 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(2-fluorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

3 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

L3 ANSWER 2 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 2006:1207230 CAPLUS
DOCUMENT NUMBER: 145:500040
TITLE: Treatment or prophylaxis of Flaviviridae viruses
using

substituted 2,3,4,9-tetrahydro-lH-carbazoles and related compounds
Gudmundsson, Kristjan
Smithkline Beecham Corporation, USA
PCT Int. Appl., 70pp.
CODEN: PIXXD2
Patent
English
1
1 INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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PA	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.			ATE	
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WO	WO 2006121466				A2 2006111			1116		WO 2	005-		20051114				
	W:	AE,	AG.	AL.	AM.	AT.	AU.	AZ.	BA,	BB,	BG,	BR.	BW.	BY,	BZ,	CA,	CH,
							DE.										
		GE.	GH.	GM.	HR.	HU.	ID.	IL.	IN.	IS.	JP.	KE.	KG.	KM,	KN,	KP,	KR.
		KZ.	LC.	LK.	LR.	LS.	LT.	LU.	LV.	LY.	MA.	MD,	MG.	MK.	MN,	MW.	MX,
		MZ.	NA,	NG,	NI,	NO,	NZ.	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,
		SG.	SK.	SL,	SM.	SY,	TJ.	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
		VN.	YU,	ZA,	ZM.	ZW											
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
		GM,	KE,	LS,	MW.	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM										

MARPAT 145:500040

The present invention relates to 2,3,4,9-tetrahydro-lH-carbazoles and related compds. (shown as 1; variables defined below: e.g. whenzyl-2,3,4,9-tetrahydrocarbazol-l-amine hydrochloride) that are

ul
in the treatment of viruses belonging to Flaviviridae, including
flaviviruses, pestiviruses, and hepaciviruses. The invention includes
compds. useful for the treatment or prophylaxis of dengue fever, yellow
fever, West Nile virus, and HCV. For I: n = 0-2; R is H or alkyl; X is
NR2, O, or S(O)m; each R! = H, halogen, haloalkyl, alkyl, alkenyl,
alkynyl, cycloalkyl, cycloalkenyl, -R1Ocycloalkyl, Ay, -NHR1OAy, Het,

ANSWER 2 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PREP (Preparation); USES (Uses)
(drug candidate; treatment or prophylaxis of Flaviviridae viruses L3

substituted 2,3,4,9-tetrahydro-lH-carbazoles and related compds.) 847988-06-1 CAPLUS 1H-Carbazol-l-amine, 6-bromo-N-(2,3-dihydro-lH-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HCl

847988-08-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride, (1s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HC1

847987-99-9P, N-Cyclohexyl-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride 847988-00-5P, N-(2,3-Dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride 847988-24-3P, N-(2,3-Dihydro-1H-inden-2-yl)-6-methyl-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride 847988-48-1P, T-Bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride 847988-48-1P, T-Bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride RL: PAC (Pharmacological activity); SPN (Synthetic preparation); USES (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

L3 ANSWER 2 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
-NHHet, -NHR10Het, -OR2, -OAy, - OHet, -R10OR2, -NR2R3, -NR2Ay,

-NHHet, -NHH10Het, -OR2, -OAy, - OHEt, -R10OR2, -NR2R3, -NR2Ay, -R10NR2R3, et al.; Y is (un) substituted alkylene, cycloalkylene, alkenylene, cycloalkenylene, or alkynylene; d = 0-1; Z is -R2, -OR2, -C(0)R2, -C(0)R2, -C(0)R2, -S(0)R2, -S(0)R2, -S(0)R2, -S(0)R2, -S(0)R2, -R10, -R10,

cycloalkyl, alkenyl, cycloalkenyl, and alkynyl; Ay = (un)substituted;

Het = (un)substituted 5- or 6-membered heterocyclyl or heteroaryl group;
addnl. details are given in the claims. Inhibition of HCV activity was
measure for 3 examples of I, e.g. IC50 = 8 nM for (IR]-6-Brome-N-(IS)-1phenylethyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine hydrochloride.
Although the methods of prepn. are not claimed, prepns. and/or
characterization data for apprx.70 examples of I are included. For
example, N-benzyl-2, 3, 4, 9-tetrahydrocarbazol-1-amine hydrochloride was
prepd. (35 % yield) by addn. of sodium triacetoxyborohydride, acetic acid
and benzylamine to a dichlorocethane soln. of 2, 3, 4, 9-tetrahydro-IHcarbazol-1-one, which was prepd. in 2 steps from 4-chloroaniline, NaNO2
and 2-(hydroxymethylene)cyclohexanone in which the intermediate
cyclohexane-1, 2-dione (4-chlorophenyl)hydrazone was cyclized.
847988-07-2, 6-Bromo-N-(2, 3-dihydro-IH-inden-2-yl)-2, 3, 4, 9tetrahydro-IH-carbazol-1-amine
RL: PEP (Physical) engineering or chemical process); PYP (Physical
process)
(chromatog, resolution; treatment or prophylaxis of Flaviviridae

using substituted 2,3,4,9-tetrahydro-1H-carbazoles and related

ompds.)

N 847988-07-2 CAPLUS

N 1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

847988-06-1P, (1R)-6-Bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4;9-tetrahydro-1H-carbazol-1-amine monohydrochloride 847988-08-3P,

-6-Bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-l-amine monohydrochloride RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

ANSWER 2 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(Uses) (drug candidate; treatment or prophylaxis of Flaviviridae viruses

y
substituted 2,3,4,9-tetrahydro-1H-carbazoles and related compds.)
847987-99-9 CAPLUS
1H-Carbazol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-, monohydrochloride
(9CI) (CA INDEX NAME)

● HCl

847988-00-5 CAPLUS |H-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

847988-24-3 CAPLUS 1H-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

(Continued) ANSWER 2 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

● HC1

847988-48-1 CAPLUS 1M-Carbazol-1-amine, 7-bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

ANSWER 3 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT:

51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L3 ANSWER 3 OF 33
CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
2006:797404 CAPLUS
145:397203
Intermolecular [4 + 2] Cycloaddition of o-Quinodimethanes Derived from Ene-Bis(sulfinylallenes)
AUTHOR(S):

AUTHOR(S):

Kitagaki, Shinjir, Katoh, Kumiko; Ohdachi, Kazuhiro; Takahashi, Yuji; Shibata, Daisuke; Mukai, Chisato Division of Pharmaceutical Sciences, Graduate School of Natural Science and Technology, Kanazawa University, Kakuma-machi, Kanazawa, 920-1192, Japan Journal of Organic Chemistry (2006), 71(18),

SOURCE: 6908-6914

CODEN: JOCEAH; ISSN: 0022-3263 American Chemical Society Journal English

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

Intermol. [4 + 2] cycloaddn. of o-quinodimethanes, prepared in situ from ene-bis(spropargylalcs.) and benzenesulfenyl chloride via ene-bis(sulfinylallene) formation, was investigated. Benzene-bridged bis(propargyl alcs.) reacted with both electron-deficient and electron-rich olefins to give the corresponding [4 + 2] cycloadducts. E.g., reaction of ene-bis(propargyl alc.) I with benzenesulfenyl chloride and di-Me fumarate, followed by oxidation with mCPRA, gave up to 844 cycloadduct II. Ethylene-bridged bis(propargyl alcs.) underwent similar cycloadduc with electron-deficient olefins. Construction of some heterocycles based on the newly developed sequential reaction is also described.

911710-49-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermol. (4 + 2] cycloaddn. of dienophiles with o-quinodimethanes prepared in situ from ene-bis(propargyl alcs.) and benzenesulfenyl chloride via ene-bis(sulfinylallene) formation)

911710-49-1 CAPLUS

91H-Benzo(b)carbazole-8,9-dicarboxylic acid, 7,8,9,10-tetrahydro-6,11-bis(phenylsulfonyl)-, dimethyl ester, (8R,9R)-rel- (9CI) (CA INDEX NAME)

L3 ANSWER 4 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2006:697809 CAPLUS COPUMENT NUMBER: 145:314757

Photo-Fries rearrangement of carbazol-2-yl

TITLE: sulfonates: efficient tool for the introduction of sulfonyl

groups

into polycyclic aromatic compounds Crevatin, Laura K.; Bonesi, Sergio M.; Erra-Balsells, AUTHOR(S):

Crevatin, Laura K.; Bonesi, Sergio M.; Erra-Balselis, Rosa
CHHIDECAR-CONICET, Departamento de Quimica Organica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, 1428, Argent.
Helvetica Chimica Acta (2006), 99(6), 1147-1157
CODEN: HCACAV; ISSN: 0018-019X
Verlag Helvetica Chimica Acta
Journal CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

AGE: Journal MAGE: English Systematic studies on the photo-Fries rearrangement of different 9H-carbazolyl sulfonates have shown that this type of conversion can be readily used for the preparative-scale introduction of alkyl- or arylsulfonyl groups into polycyclic aromatic compds. under very mild conditions. A series of new 1-sulfonyl- or 3-sulfonyl-9H-carbazole derivs. were prepared in medium-to-good yields, and characterized by Ss.

15, 1H-NMR, and 13C-NMR spectroscopy, as well as by elemental anal. Effects of irradiation wavelength, solvent polarity, presence or absence of O2,

photosensitizers were studied in detail. For example, the rearrangement of -9H-carbazol-2-ol methanesulfonate (ester) gave 1-(methylsulfonyl)-9H-carbazol-2-ol (major product) and 3-(methylsulfonyl)-9H-carbazol-2-ol. 908850-23-7P

IT 908850-23-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (sulfonyl)carbazolol derivs. Via regioselective
photo-Fries
rearrangement of carbazolol sulfonate esters)
RN 908850-23-7 CAPLUS
CN 9H-Carbazol-2-ol, 1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: THIS

THERE ARE 44 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2006:608619 CAPLUS DOCUMENT NUMBER: 145:83213 ACCESSION NUMBER DOCUMENT NUMBER: TITLE: 145:83213
Preparation of tetrahydrocarbazoles as active agents for inhibiting VEGF production by translational control Lennox, William Joseph; Qi, Hongyan; Lee, Duck-Hyung; Choi, Soongyu; Moon, Young-Choon PTC Therapeutics, Inc., USA PCT Int. Appl., 137 pp. CODEN: PIXXD2
Patent English
3 INVENTOR (S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE A2 200660622 W0 2005-U542483
A3 200660803
AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, CU, CZ, DE, DK, DM, DZ, EC, EZ, EG, ES, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, LK, LS, LT, LU, LV, LY, MA, MD, MG, MK, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, 2M, ZW, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, CM, GA, GO, GW, ML, MR, NE, SN, TD, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, RU, TJ, TM WO 2006055490

WO 2006055490

W: AE, AG, AL,
CN, CO, CR,
GE, GH, GM,
KZ, LC, LK,
MZ, NA, NG,
SG, SK, SL,
VN, YU, ZA,
RW: AT, BE, BG,
IS, IT, LT,
CF, CG, CI,
GM, KE, LS,
KG, KZ, MD,
PRIORITY APPLN. INFO.: 20051123 BZ, CA, CH, FI, GB, GD, KN, KP, KR, MN, MW, MX, SC, SD, SE, US, UZ, VC, DK, EE, ES, FI, FR, GB, GR, HU, IE, PL, PT, RO, SE, SI, SK, TR, BF, BJ, GW, ML, MR, NE, SN, TD, TG, BW, GH, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, P 20041123 US 2004-633738P P 20041206

US 2004-639283P

OTHER SOURCE(S): MARPAT 145:83213

P 20041227

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

III

The present invention relates to methods, compds., and compns. for inhibiting angiogenesis. More particularly, the present invention ${\bf r}$ to methods, compds., and compns. for inhibiting VEGF production The

compds. I {X = NR9R10, N(alkyl)C(0)aryl, H, etc. (wherein R9, R10 = H, alkyl, aryl, etc.; or NR9R10 = mono- or bicyclic heterocyclic ring);

alkyl, aryl, etc.; or NR9R10 = mono- or bicyclic heterocyclic ring);
R1-R3
R1-

production by translational control) 812649-13-1 CAPLUS HH-Carbasol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA NAME)

ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-16-4P 812649-17-5P 812649-20-0P
812649-21-1P 812649-22-2P 812649-46-0P
812649-47-1P 812649-49-3P 812649-50-6P
812649-47-1P 812649-52-8P 812649-53-9P
812645-51-7P 812649-52-8P 812649-53-9P
814255-12-4P 814255-18-0P 893409-63-7P
893409-67-1P 893409-69-3P 893409-71-7P
893409-75-1P 893409-82-0P 893409-71-7P
893409-19-5P 893409-82-0P 893409-83-1P
893409-86-8P 893409-39-2P 893409-86-6P
893409-86-8P 893409-31-3P 893409-86-6P
893409-86-5P 893410-00-1P 893410-10-1P
893410-65-P 893410-61-2P 893410-10-1P
893410-63-4P 893410-64-5P
893410-63-4P 893410-64-5P
893410-63-4P 893410-64-5P
893410-63-4P 893410-61-2P 893410-62-3P
893410-63-4P 893410-61-2P 893410-62-3P
893410-63-4P 893410-61-5P 893410-61-3P
893410-63-4P 893410-61-5P 893410-62-3P
893410-63-4P 893410-61-5P 893410-82-3P
893410-893410-81-4P 893410-81-4P
893410-893410-81-4P
893410-893410-81-4P
893410-893410-81-4P
893410-893410-81-4P
893410-81-4P
893410-81-

(preparation of tetrahydrocarbazoles as active agents for inhibiting

production by translational control)
812649-16-4 CAPLUS
1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)(9CI) (CA INDEX NAME)

812649-17-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4-chlorophenyl)-2,3,4,9-tetrahydro-(CA INDEX NAME)

ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-20-0 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-(CA INDEX NAME)

812649-21-1 CAPLUS 1H-carbazol-1-amine, 6-bromo-N-(4-chlorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-22-2 CAPLUS .
1H-Carbazol-1-amine, 6-bromo-N-(4-fluorophenyl)-2,3,4,9-tetrahydro- (9CI)

ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (CA INDEX NAME)

812649-46-0 CAPLUS
'1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(3-methoxyphenyl)-RN CN (9CI)

812649-47-1 CAPLUS IH-Carbazol-1-amine, 6-bromo-N-(3-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

NASWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 812649-52-8 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(3,4-dichlorophenyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

812649-53-9 CAPLUS 1H-Carbazole, 6-bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro- {9CI} (CA INDEX NAME)

814255-12-4 CAPLUS 1H-Carbacol-lamine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

814255-18-0 CAPLUS

ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 812649-49-3 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(2-methoxyphenyl)-L3 I RN I CN (9CI) (CA INDEX NAME)

812649-50-6 CAPLUS 1H-Carbazol-1-emine, 6-bromo-N-(2-chlorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-51-7 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-{2-fluorophenyl}-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethyl)-(9CI) (CA INDEX NAME)

893409-63-7 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[4-{trifluoromethyl}phenyl]- (9CI) (CA INDEX NAME)

893409-67-1 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[4-(1-methylethyl)phenyl)- (9CI) (CA INDEX NAME)

893409-69-3 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-{4-phenoxyphenyl}-(CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

oph NH H H N Br

RN 893409-71-7 CAPLUS CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-phenyl- (9CI) (CA INDEX NAME)

NHPh H N Me

RN 893409-75-1 CAPLUS
CN 1H-Carbazol-1-amine, N-1,3-benzodioxol-5-yl-6-bromo-2,3,4,9-tetrahydro(9C1) (CA INDEX NAME)

RN 893409-76-2 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2, 3, 4, 9-tetrahydro-N-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Ph NN H NN Br

Ph NH H NN B

RN 893409-85-3 CAPLUS (NH-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-pyrazinyl- (9CI) (CA INDEX NAME)

NH H

RN 893409-86-4 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(2,3-difluorophenyl)-2,3,4,9-tetrahydro(9C1) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

F3C-0

RN 893409-77-3 CAPLUS
CN 1H-Carbazol-l-amine, 6-bromo-N-(3-chlorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA TNDEX NAME)

C1 NH H

RN 893409-79-5 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(3,5-dimethylphenyl)-2,3,4,9-tetrahydro(9CI) (CA INDEX NAME)

RN 893409-82-0 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(4-phenylcyclohexyl)(9CI) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

F NH H

RN 893409-87-5 CAPLUS CN Cyclohept(b)indol-6-amine, 2-bromo-5,6,7,8,9,10-hexahydro-N-phenyl- (9CI) (CA INDEX NAME)

NHPh H N N B

RN 893409-88-6 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-{trifluoromethoxy}-{9Cl} '{CA INDEX NAME}

O-CF3

RN 893409-93-3 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[4-(4-morpholiny1)pheny1]- (9CI) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 893409-96-6 CAPLUS
CN 1H-Carbazol-1-amine, 5-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

RN 893409-97-7 CAPLUS

Senzonitrile, 4-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)amino](9CI) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN · (Continued) dimethyl- (9C1) (CA INDEX NAME)

RN 893410-10-1 CAPLUS
CN Benzeneethanol, 3-((6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)aminol-(9C1) (CA INDEX NAME)

RN 893410-32-7 CAPLUS CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-1H-pyrrol-1-yl- (9CI) (CA INDEX NAME)

RN 893410-61-2 CAPLUS
CN 1H-Carbazo1-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-[4-(trifluoromethyl)phenyl)- (SCI) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 893409-99-9 CAPLUS
CN 1H-Carbazol-1-amine, 7-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA
INDEX
NAME)

RN 893410-02-1 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-3-isoxazolyl- (9CI) (CA INDEX NAME)

RN 893410-06-5 CAPLUS
CN Acetamide, N-[4-((6-bromo-2,3,4,9-tetrahydro-lH-carbazol-1-yl)amino]phenyl]- (9CI) (CA INDEX NAME)

RN 893410-08-7 CAPLUS
CN 1,4-Benzenediamine, N'-(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)-N,N-

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 893410-62-3 CAPLUS
CN 1H-Carbazol-l-amine, N-(4-chlorophenyl)-2,3,4,9-tetrahydro-6(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 893410-63-4 CAPLUS
CN IH-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-6(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 893410-64-5 CAPLUS
CN IH-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-(trifluoromethyl)-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

IT

118498-97-8 471259-01-5 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (preparation of tetrahydrocarbazoles as active agents for inhibiting

VEGE

production by translational control)
118498-97-8 CaPLUS
1H-Carbazol-1-amine, N-cyclohexyl-2, 3, 4, 9-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)

471259-01-5 CAPLUS

H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-nitro-N-(4-phenylcyclohexyl)-(9CI) (CA INDEX NAME)

L3 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

L3 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:404930 CAPLUS
DOCUMENT NUMBER: 145:465900 F.
TITLE: Reactions of the melatonin metabolite
N1-acetyl-5-methoxykynuramine (AMK) with the ABTS
cation radical: identification of new oxidation
products

cation radical: identification of new exidation products

AUTHOR(S): Than, Ni Ni; Heer, Christina; Laatsch, Hartmut; Hardeland, Ruediger

CORPORATE SOURCE: Institutes of Organic and Biomolecular Chemistry, University of Goettingen, Goettingen, Germany

SOURCE: Redox Report (2006), 11(1), 15-24

CODEN: RDRPE4; ISSN: 1351-0002

URL:

http://www.ingentaconnect.com/content/maney/rer/2

OG6/0000001/0000001

PUBLISHER: Maney Publishing

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB The melatonin metabolite N1-acetyl-5-methoxykynuramine (AMK; 1), which was

previously shown to be a potent radical scavenger, was oxidized using the ABTS cation radical [ABTS = 2,2'-azinobis-(3-ethylbenzthiazoline-6-sulfonic acid)] Several new oxidation products were obtained, which

separated by repeated chromatog. and characterized by spectroscopic

such as mass spectrometry (ESI-MS and ESI-HRMS), 1H-NMR and 13C-NMR,

HSQC, H,H COSY correlations and IR spectroscopy. The main products were oligomers of 1 (3 dimers, 1 trimer and 2 tetramers). In all cases, the amino group N2 was involved in the reactions. Two of the dimers turned out to be cis (2a) and trans (2b) isomers containing an ato bond. In the other dimer (3a), the nitrogen stom N2 was attached to atom C5 of the second aromatic amine, with loss of the methoxy group. In the trimer,

N2 formed a bridge to C5 of unit B, as in the resp. dimer, while this one of C had bridged to C6 of B. One of the tetramers was composed of a trimer 5 attached to N2 of a fourth 1 mol. via an azo bond as in 2a/b.

the other tetramer, an addnl. C-C bond between rings B and C in 6 is assumed. Although oligomers of AMK may only attain low in vivo concns., the types of reactions observed shed light on the physiol. possible metabolism of

AMK once reacted with a free radical. The displacement of a methoxy group, rarely seen in the oxidation of methoxylated biomols., underlines

reactivity of AMK. Preliminary data show that, in the presence of ABTS cation radicals, AMK can interact with side chains of aromatic amino

cation radicals, ANK can interact with side chains of aromatic amino acids, a finding which may be crucial for understanding to date unidentified protein modification by a melatonin metabolite detected earlier in expts. with radioactively labeled melatonin.

IT 914087-91-5

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL

RE: BSO (DIODICAL SEMBY, unclassified), FAF (Flopetices), BSO (Biological study) (reactions of melatonin metabolite NI-acetyl-5-methoxykynuramine (AMK) with ABTS cation radical and identification of new oxidation products) 914087-91-5 CAPLUS

Acetamide, N,N'-{[8-[[2-[3-(acetylamino)-1-oxopropy1]-4-

ANSWER 6 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) methoxyphenyl]amino]-5-[{2-[3-(acetylamino]-1-oxopropyl]-4-methoxyphenyl]aro]-3-methoxy-9H-carbazole-1,6-diyl]bis(3-oxo-3,1-propanediyl]]bis(3CI) (CA INDEX NAME)

37

REFERENCE COUNT:

THERE ARE 37 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ACCESSION NUMBER:
DOCUMENT NUMBER:
144:369846
Synthesis and SAR of substituted tetrahydrocarbarole derivatives as new NPY-1 antagonists
AUTHOR(S):

DI Fabio, Romano; Giovannini, Riccardo; Bertani, Barbara; Borriello, Manuela; Bozzoli, Andrea; Donati, Daniele; Falchi, Alessandro; Ghirlanda, Damiano; Leslie, Colin P.; Pecunicoo, Angelo; Rumboldt, Giovanna; Spada, Simone
Glavosmithkline Medicines Research Centre, Verona, 37135, Italy
Bioorganic & Medicinal Chemistry Letters (2006), 16(6), 1749-1752
COEDE: BMCLE8; ISSN: 0960-894X
Elsevier B.V.
Journal
LANGUAGE: CASREACT 144:369846

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

The SAR of a new series of tetrahydrocarbazole derivs. I [Rl = Me, 3-(1-piperidiny1)propy1, piperidin-4-ylmethy1, etc.; R2 = H, 4-morpholiny1, 1-piperidiny1, 4-methy1-1-piperaziny1, etc.] is evaluated: the appropriate decoration of this template led to the identification of

new class of NPY-1 antagonists showing good in vitro potency and a promising in vivo pharmacokinetic profile in rat. 882033-76-3P 882033-77-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and SAR of amino(chlorophenoxy)tetrahydrocarbazolones as IT

NPY-1

antagonists)
882033-76-3 CAPLUS
1H-Carbazole, 1-(4-chlorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA INDEX
NAME)

ACCESSION NUMBER: DOCUMENT NUMBER: TITLE:

AUTHOR (S):

CORPORATE SOURCE: SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

ANSWER 8 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN
ESSION NUMBER: 2005.444285 CAPLUS

LE: Effects of fluorination on electronic and excited

STATES OURCE: STATES OF STA

the increasing number of porphyrins compared to the unfluorination and

other types of fluorinations. It is found that the infinite fused fluorinated ZnP tapes with narrow gap (=0.1 eV-0.2 eV) as predicted by using the periodic-DFT level are slightly inferior to the near-zero gap semimetallic unfluorinated ZnP tape as a conducting mol. wire. The combination of the condensation and the meso- and/or \(\theta\)-fluorination of ZnP can finely tune the LUMO level to the Fermi level of the electrodes for fabrication of n-type conducting materials. The fused fluoro-oligoporphyrins may then become new n-type organic semiconductors, provided they are well crystallized with a high electron mobility, such as the recently synthesized perfluoropentacene.

859507-60-1
RI: FEP (Physical, engineering or chamical armounts)

IT RL: PEP (Physical, engineering or chemical process); PRP (Properties);

(Physical process): PROC (Process)
(comparison: fluorination effect on electronic and excited states of fused zinc oligoporphyrins in relation to)
859507-60-1 CAPLUS
Poly(5,15-difluoro-21H,23H-porphine-2,18,20:8,10,12-hexayl-kN21,kN22,kN23,kN24 (SP-4-1)-zinc complex) (9CI)
(CA INDEX NAME)

L3 ANSWER 7 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

882033-77-4 CAPLUS
4H-Carbazol-4-one, 1-(4-chlorophenoxy)-1,2,3,9-tetrahydro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

61

REFERENCE COUNT:

THERE ARE 61 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 200503791 Al 20050428 WO 2004-US34169 20041015

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, VU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, MA, SD, SL, SZ, TZ, UG, ZM, ZW, AW, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, CM, SM, CE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SM, TD, TG

EP 1678137 Al 20060712 EP 2004-795347 20041015

R: AT, BE, CH, DZ, DX, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, FRIORITY APPIN. INFO::

WO 2004-US34169 W 20041015

OTHER SOURCE(S): MARPAT 142:430133

AB Title compds. I [R1 = H, halo, formyl, etc.; R2 = heteroaryl, arylalkyl, alkyl, etc.; R7 = H, NHZ, alkyl, etc.; R9 = H, alkyl; n = 1-4; p = 0-2] and their pharmaceutically acceptable salts were prepared For example, reductive amination of 6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-one,

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 419576-59-3 CAPLUS CN 1H-Carbazol-1-amine, N-(1-ethyl-4-piperidinyl)-2,3,4,9-tetrahydro-6-nitro-(SCI) (CA INDEX NAME)

RN 471259-03-7 CAPLUS CN 1H-Carbazol-1-amine, N-bicyclo[2.2.1]hept-2-yl-2,3,4,9-tetrahydro-6-nitro-{9CI} (CA INDEX NAME)

RN 851054-01-8 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-N-cyclohexyl-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME) ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) prepd. from 4-bromoaniline, with cyclohexylamine afforded 6-bromo-N-cyclohexyl-2,3,4,9-tetrahydro-1H-carbazole-1-amine (II). In inhibition assays, compd. II·CF3CO2H showed activity at <4 µM. Compds. I are claimed useful for the treatment of HCV, SARS, etc. I 18498-97-88 419576-59-19 471259-03-77 81054-01-88 851054-02-9P 851054-03-0P 851054-48-3P 851054-48-3P 851054-47-2P 851054-48-3P 851054-47-2P 851054-48-3P 851054-47-2P 851054-48-3P 851054-48-3P 851054-48-3P 851054-58-3P 851054-53-0P 851054-53-0P 851054-53-0P 851054-53-0P 851054-53-0P 851054-89-3P 851054-89-3P 851054-89-3P 851054-98-3P 851055-19-9P 851055-03-P 851055-03-P 851055-03-P 851055-03-P 851055-03-P 851055-03-P 851055-10-2P 851055-11-3P 851055-12-4P 851055-12-4P 851055-12-4P 851055-12-4P 851055-12-4P 851055-13-4P 851055-12-4P 851055-13-4P 851055-13-4P 851055-13-4P 851055-14-6P 851055-13-4P 851055-14-6P 851055-13-4P 851055-13-4P 851055-14-6P 851055-13-4P 851055-14-6P 851055-13-4P 851055-14-6P 851055-13-4P 851055-13-4P 851055-34-4P 851055-35-4P 851055-34-4P 851055-35-4P 851055-34-4P 851055-35-4P 851055-34-4P 851055-35-4P 851055-35-4P 851055-34-4P 851055-35-4P 851056-03-4P 851056

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851054-02-9 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-cyclohexyl-2,3,4,9-tetrahydro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 851054-01-8 CMF C18 H23 Br N2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 851054-03-0 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

851054-04-1 CAPLUS
1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(phen)lmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-methyl- (9CI) (CA INDEX NAME)

RN 851054-29-0 CAPLUS CN HH-Carbazole-6-methanamine, 1-(cyclohexylamino)-N-ethyl-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

851054-30-3 CAPLUS IH-Carbazole-6-carboxylic acid, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

851054-39-2 CAPLUS

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 851054-08-5 CAPLUS H-Carbazol-1-amine, N-cyclohexyl-6-fluoro-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

851054-13-2 CAPLUS IN-Carbazol-1-amine, 6-chloro-N-cyclohexyl-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

851054-18-7 CAPLUS
1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-methyl- (9CI) (CA INDEX NAME)

851054-28-9 CAPLUS

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2, 3, 4, 9-tetrahydro-N-2-propenyl- (SCI) (CA INDEX NAME)

RN 851054-41-6 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-N-ethyl-2,3,4,9-tetrahydro{9CI} (CA INDEX NAME)

851034-42-7 CAPLUS IN-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(1-methylethyl)- (9C1) (CA INDEX NAME)

851054-46-1 CAPLUS 1H-Carbarol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-(2-pyridinyl)-(SC1) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

NH H

RN 851054-47-2 CAPLUS
CN 1H-Carbazol-l-amine, N-cyclohexyl-2, 3, 4, 9-tetrahydro-6-(3-pyridinyl)(9C1) (CA INDEX NAME)

MH H

RN 851054-48-3 CAPLUS
CN 1H-Carbazol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-{4-pyridinyl}{9Cl} (CA INDEX NAME)

NH H

RN 851034-49-4 CAPLUS
CN HH-Carbazol-1-amine, 7-bromo-N-cyclohexyl-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H N C-NHEL

RN 851054-56-3 CAPLUS
CN 1H-Carbacel-6-carboxamide, N-ethyl-2,3,4,9-tetrahydro-1-[[4-methylcyclohexyl]amino]- [SCI] (CA INDEX NAME)

MH H H C-NHEt

RN 851054-57-4 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

C-NHPr-1

RN 851054-59-6 CAPLUS

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

NH H Br

RN 851054-50-7 CAPLUS
CN 1H-Carbazol-1-amine, 8-bromo-N-cyclohexyl-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

NH Br

RN 851054-53-0 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-2-propenyl- (9CI) (CA INDEX NAME)

C-NH-CH₂-CH=CH₂

RN 851054-55-2 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cycloheptylamino)-N-ethyl-2,3,4,9tetrahydro- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Carbacele--methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-methoxyethyl)- (9C1) (CA INDEX NAME)

NH H

CH2-NH-CH2-CH2-OMe

RN 851054-66-5 CAPLUS
CN Cyclobutanecarboxamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazo1-6-yl]- (9C1) (CA INDEX NAME)

NH H

RN 851054-67-6 CAPLUS
CN IH-Carbazol-l-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-(1-piperidinylmethyl)- (9CI) (CA INDEX NAME)

NH H CH2-N

RN 851054-71-2 CAPLUS
CN 1H-Carbazol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-(4-morpholinylmethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851054-75-6 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-{cyclohexylamino}-2,3,4,9-tetrahydro-N-{2-methoxyethyl}- {9Cl} (CA INDEX NAME)

RN 851054-84-7 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-N-(2-furanylmethyl)2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851054-86-9 CAPLUS
CN Cyclopentanecarboxamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1Hcarbazol-6-yll- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851054-93-8 CAPLUS

1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2, 3, 4, 9-tetrahydro-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 851054-94-9 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 851054-96-1 CAPLUS
CN 1H-Carbazole-6-carboxamide, N-cyclohexyl-1-(cyclohexylamino)-2,3,4,9-tetrahydro- (SCI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851054-87-0 CAPLUS
CM 1H-Carbazole-6-methanamine, N-cyclohexyl-1-(cyclohexylamino)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851054-88-1 CAPLUS
CN | H-Carbazole-6-methanamine, | 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(tetrahydro-2-furanyl)methyl| - (9Cl) (CA INDEX NAME)

RN 851054-92-7 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851054-97-2 CAPLUS
CN Cyclopentaneacetamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1Hcarbazol-6-yl]- (9CI) (CA INDEX NAME)

RN 851054-98-3 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-N-(cyclohexylmethyl)2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851054-99-4 CAPLUS
CN | H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N[[(2R)-tetrahydro-2-furanyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-00-0 CAPLUS
CN | H-Carbarole-6-carboxamide, | 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N[(cetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

RN 851055-01-1 CRPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N[[(2S)-tetrahydro-2-furanyl]methyl]- [9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 851055-10-2 CAPLUS
CN 1H-Carbazole-6-methanamine,
1-(cyclohexylamino)-N-[(4-fluorophenyl)methyl)2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851055-11-3 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-thienylmethyl)- (9CI) (CA INDEX NAME)

RN 851055-12-4 CAPLUS
CN HH-Carbazole-6-carboxemide, 1-(cyclohexylamino)-N-(cyclohexylmethyl)2,3,4,9-tetrahydro- (9C1) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 851055-05-5 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 851055-06-6 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-pyridinylmethyl)- (9Cl) (CA INDEX NAME)

RN 851055-07-7 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 851055-08-8 CAPLUS

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-13-5 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-(1-pyrrolidinyl)ethyl)- (9CI) (CA INDEX NAME)

RN 851055-14-6 CAPLUS CN Benzamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]-2,4dimethyl- (9CI) (CA INDEX NAME)

RN 851055-15-7 CAPLUS
CN Benzenepropanamide,
N-(1-(cyclohexylamino)-2,3,4,9-tetrehydro-1H-carbazol-6-yl)-(9CI) (CA INDEX NAME)

(Continued)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-16-8 CAPLUS
CN IH-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 851055-17-9 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 851055-18-0 CAPLUS
CN 1H-Carbazole-6-carboxamide, 2,3,4,9-tetrahydro-1-[(4-methylcyclohexyl)aminoj-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 851055-27-1 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-[2-(4morpholinyl)ethyl)- (9CI) (CA.INDEX NAME)

RN 851055-31-7 CAPLUS
CN IH-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(3-phenylpropyl)- (9C1) (CA INDEX NAME)

RN 851055-32-8 CAPLUS
CN Benzeneacetamide,
N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6y1]-2,4-dimethyl- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-21-5 CAPLUS
CN Benzeneacetamide,
N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6yl]-4-fluoro- (9CI) (CA INDEX NAME)

RN 851055-22-6 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-N-[2-(4-fluorophenyl)ethyl]-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851055-23-7 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-{2-{1-

NH H Me

RN 851055-33-9 CAPLUS
CN Benzenebutanamide,
N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6yl]- (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

RN 851055-34-0 CAPLUS

1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-(4-phenylbutyl)- (961) (CA INDEX NAME)

RN 851035-37-3 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-[(4-methoxyphenyl)methyl]- [9CI] (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-38-4 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-N-[2-(4-fluorophenyl)ethyl]-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851055-41-9 CAPLUS CN 1H-Carbazole-6-carboxamide, 1-{cyclohexylamino}-2,3,4,9-tetrahydro-N-[3-(2oxo-1-pyrrolidinyl)propyl}- (9CI) (CA INDEX NAME)

RN 851055-50-0 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-N-([4-(dimethylamino)phenyl]methyl]-2,3,4,9-tetrahydro-(SCI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-63-5 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 851055-70-4 CAPLUS
CN IH-Carbazole-6-carboxamide, 1-(cyclohexylamino)-N-[2-[2-[2-[[5-[[3-[4,4,6,6as]-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]ethoxy]ethoxy]ethyl]-2,3,4,9-tetrahydro- (9CI)
NAME)

Absolute stereochemistry.

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851055-51-1 CAPLUS CN Benzamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-y1]-2,4dimethoxy- (9CI) (CA INDEX NAME)

RN 851055-54-4 CAPLUS
CN Benzamide, N-{1-(cyclohexylamino)-2,3,4,9-tetrahydro-lH-carbazol-6-yl}-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 851055-55-5 CAPLUS
CN 1H-Carbazole-6-methanamine, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

PAGE 1-B

RN 851055-75-9 CAPLUS
CN Cyclopent[b]indol-3-amine, N-cyclohexyl-1,2,3,4-tetrahydro-7-methyl(9CI)
(CA INDEX NAME)

RN 851055-79-3 CAPLUS CN 1H-Carbazole-6-carboxylic acid, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

RN 851055-80-6 CAPLUS CN 1H-Carbazol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-phenyl- (9CI) (CA INDEX NAME) L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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RN 851055-88-4 CAPLUS CN H-Carbazole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851055-91-9 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cycloheptylamino)-2,3,4,9-tetrahydro-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 851055-98-6 CAPLUS CN 1H-Carbazole-6-carboxamide, 1-(cyclopentylamino)-N-ethyl-2,3,4,9-

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

RN 851056-02-5 CAPLUS
CN Piperazine, 1-[(1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 851056-03-6 CAPLUS
CN Piperidine, 1-[[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yllcarbonyll-(GCI INDEX NAME)

RN 851056-04-7 CAPLUS
CN Pyrcolidine, 1-[[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yllcarbonyl]- (GK) (CA INDEX NAMZ)

RN 851056-05-8 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-M-ethyl-2,3,4,9-tetrahydroN-methyl- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) tetrahydro- (9CI) (CA INDEX NAME)

RN 851056-00-3 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-N-[2-(dimethylamino)ethyl]2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 851056-01-4 CAPLUS
CN 1H-Carbazole-6-carboxamide,
1-(cyclohexylamino)-2,3,4,9-tetrahydro-N-{3-(4-morpholinyl)propyl}- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN . (Continued)

RN 851056-06-9 CAPLUS
CN 1H-Carbazole-6-carboxamide, 1-(cyclopentylamino)-2,3,4,9-tetrahydro-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 851056-10-5 CAPLUS
CN Morpholine, 4-[[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]carbonyl)- (9CI) (CA INDEX NAME)

RN 851056-14-9 CAPLUS CN Cyclopropaecarboxamide, N-{1-(cyclohexylamino)-2,3,4,9-tetrahydro-1Hcarbazol-6-yl]- (9CT) (CA INDEX NAME) L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 851056-15-0 CAPLUS
CN Propanamide,
N-(1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]-2methyl- (9CI) (CA INDEX NAME)

851056-16-1 CAPLUS Benzamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]-2-fluoro-(9CI) (CA INDEX NAME)

851056-17-2 CAPLUS 2-Pyridinecarboxamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-lH-carboxol-6-yl)- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

851056-21-8 CAPLUS
3-Pyridinecarboxamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-lH-carbox01-6-yl]- (9CI) (CA INDEX NAME)

RN 851056-22-9 CAPLUS
CN 1H-Carbazole-6-methanamine,
1-(cyclohexylamino)-M-ethyl-2,3,4,9-tetrahydroN-methyl- (9CI) (CA INDEX NAME)

851056-23-0 CAPLUS
1H-Carbazol-1-amine, N-cyclohexyl-2, 3, 4, 9-tetrahydro-6-(1-pyrrolidinylmethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

851056-18-3 CAPLUS
Benzeneacetamide, 4-bromo-N-(1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl)- (9CI) (CA INDEX NAME)

RN 851056-19-4 CAPLUS CN [1,1'-Biphenyl]-4-acetamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]- (9CI) (CA INDEX NAME)

851056-20-7 CAPLUS Butanamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl]-(SCI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

851056-24-1 CAPLUS
1H-Carbazol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-[(4-methyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)

851056-25-2 CAPLUS 2-Pyrrolidinone, 1-[3-[[[1-(cyclohexylamino)-2,3,4,9-tetrahydro-lH-carbazol-6-yl]methyl]amino|propyl]- (9CI) (CA IMDEX NAME)

851056-26-3 CAPLUS
4-Pyridinecarboxamide, N-{1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbox01-6-y1|- (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

HH-Carbacole-6-carboxamide, 1-(cyclohexylamino)-2,3,4,9-tetrahydro-N,N-dimethyl- (9CI) (CA INDEX NAME)

851056-28-5 CAPLUS
Propanamide, N-[1-(cyclohexylamino)-2,3,4,9-tetrahydro-1H-carbazol-6-yl][9C1] (CA INDEX NAME)

031036-29-6 CAPLUS IH-Carbazole-1,6-diamine, N1-cyclohexyl-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME) 851056-29-6

L3 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2007 ACS On STN
ACCESSION NUMBER: 2005:232610 CAPLUS
DOCUMENT NUMBER: 142:316689
Preparation of novel cycloalkyl[b] condensed indoles for treating human papillomaviruses
Boggs, Sharon Davis: Catalano, John G.; Gudmundsson, Kristjan S.; D'Aurora Richardson, Leah; Sebahar, Paul Richard
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
PCT Int. Appl., 89 pp.
COODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

P	ATENT	ΝО.			KIND DATE						DATE						
											2004-						
	W:	AE.	AG.	AL,	AM.	AT.	AU,	AZ,	BA,	ВВ	, BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN.	co.	CR.	CU.	CZ.	DE.	DK,	DM,	DZ	, EC,	EE,	EG,	.ES,	FI,	GB,	GD,
		GE.	GH.	GM.	HR.	HU,	ID,	IL.	IN,	18	, JP,	KE,	KG,	KP,	KR,	KZ,	LC,
											, MK,						
		NO.	NZ.	OM.	PG.	PH.	PL.	PT.	RO,	RU	, sc,	SD,	SE,	SG,	SK,	SL,	SY,
											, UZ,						
	RW:	BW.	GH,	GM,	KE,	LS,	MV.	MZ,	NA,	SD	, SL,	SZ,	т2,	UG,	ZM,	ZW,	AM,
		AZ.	BY.	KG,	KZ,	MD,	RU,	TJ,	TM,	AT	, BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE.	ES.	FI.	FR.	GB,	GR,	HU,	IE.	IT	, LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI.	SK.	TR.	BF.	BJ,	CF.	CG,	CI,	CM	, GA,	GN,	GQ,	GW,	ML,	MR,	NE,
			TD.														
E	1658	068			Al		2006	0524		EΡ	2004-	7545	53		2	0040	607
_											, IT,						
		IE.	SI.	LT.	LV.	FI.	RO.	CY.	TR.	BG	, cz,	EE.	HU,	PL,	SK,	HR	
J	2007	5034	34		T		2007	0222		JΡ	2006-	5246	21		2	0040	607
U	2006	2818	04		A1		2006	1214		US	2006-	5695	24		2	0060	224
PRIORI'	TY APP	LN.	INFO	.:						US	2003-	4978	45P		P 2	0030	826
										ΨO	2004-	11917	982		w 2	0040	607

MARPAT 142:316689

The present invention relates to cycloalkyl(b) condensed indoles (shown I; variables defined below; e.g. 6-chloro-2, 3, 4, 9-tetrahydro-1H-carbazol-1ANSWER 9 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) amine), including administration of pharmaceutically acceptable salts, solvates, and physiol. functional derivs. thereof, that are useful in the treatment of human papillomaviruses (HPVs), and also to the methods for the making and use of such compds. HPV inhibition values for 56 examples of I are reported. For I: n = 0-2; R is H or alkyl; X is NR2, O, or S(O)m; each R1 = H, halogen, haloalkyl, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, R10cycloalkyl, Ay, NHR10Het, OR2, OAy, OHet, R10ORZ, NR2A3, NR2AY, R10RYR2AY, R10RYR2AY, R10C(O)R2, CO2R2, R10CO2R2, C(O)NR2R3, C(O)NR2AY, C(O)NR2AY, Het.

C(O) Het

are
not claimed, .apprx.70 example prepns. are included. For example,
6-chloro-2,3,4,9-tetrahydro-1H-carbazol-1-amine was prepd. (52 %) from
6-chloro-2,3,4,9-tetrahydro-1H-carbazol-1-one, NH4OAc, and NaBH3CN in
MeOH; the ketone was prepd. (88 %) by cyclization of
cyclohexane-1,2-dione
(4-chlorophenyl)hydrazone, which was prepd. (49 %) from the diazonium
salt

salt
of 4-chloroaniline and 2-(hydroxymethylene)cyclohexanone.

IT 847988-07-2, 6-Bromo-N-[2,3-dthydro-lH-inden-2-yl)-2,3,4,9tetrahydro-lH-carbazol-l-amine
RL: PPP [Physical: engineering or chemical process): PYP (Physical
process): PROC (Process)
(chromatog. resolution; preparation of novel cycloalkyl{b} condensed
indoles

for treating human papillomaviruses)
847988-07-2 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9tetrahydro- (9CI) (CA INDEX NAME)

84798B-06-1P, (1R)-6-Bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine hydrochloride 847988-08-3P,

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
1-amine hydrochloride
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(drug candidate; prepn. of novel cycloalkyl[b] condensed indoles for
treating human papillomaviruses)
847988-06-1 CAPLUS
HH-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9tetrahydro-, monohydrochloride, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

847988-08-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-, monohydrochloride, (IS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HC1

847987-99-9P, N-Cyclohexyl-2,3,4,9-tetrahydro-1H-carbazol-1-amine hydrochloride 847988-00-5P, N-(2,3-Dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine hydrochloride 847988-24-3P

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

847988-48-1 CAPLUS 1H-Carbarol-1-amine, 7-bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-, monohydrochloride (9CT) (CA INDEX NAME)

REFERENCE COUNT:

FORMAT

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L3 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

• HCl

.
847988-00-5 CAPLUS
1H-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-,
monohydrochloride (9CI) (CA INDEX NAME)

• HC1

847988-24-3 CAPLUS IH-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1127334 CAPLUS
1117-127445 1127-1445
INVENTOR(S): Began applilomaviruses inhibitors
Boggs, Sharon Davis; Gudmundsson, Kristjan S.;
Richardson, Leah D'Aurora: Sebahar, Paul Richard
SOURCE: STREET ASSIGNEE(S): STREET ASSIGNEE (S): PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Pateri

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	TENT	ю.			KIND DATE												
WO	WO 2004110999						20041223			WO 2004-US17660							
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
											EC,						
		GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	ıs,	J₽,	ΚE,	KG,	ΚP,	KR,	ΚŻ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	ΜX,	MZ,	ΝA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	vc,	VN,	YU,	ZA,	ZM,	ZW
	RW:										SL,						
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	TG													
AU	2004	2476	76		A1		2004	1223		AU 2	004-	2476	76		2	0040	607
CA	2528	321			A1		2004	1223		CA Z	004-	2528	321		2	0040	607
EP	1654	228			A1		2006	0510		EP 2	004-	7762	79		2	0040	607
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR	
BR	2004	0110	85		A		2006	0725		BR 2	004-	1108	5		2	0040	607
CN	1832	921			A		2006	0913		CN 2	004-	8002	2227		2	0040	607
JP	2007	5012	84		T		2007	0125		JP 2	006-	5335	61		2	0040	607
NO	2005	0057	41		A		2006	0106		NO 2	005-	5741			2	0051	205
US	2006	1610	02		Al		2006	0720		ŲS 2	005-	5600	13		2	0051	208
PRIORITY	2004 1832 2007 2005 2006 APP	LN.	INFO	.:						US 2	003-	4772	51P	1	P 2	0030	610
										US 2	003-	4978	23P	1	P 2	0030	826
										WO 2	004-	US17	660	,	W 2	0040	607

OTHER SOURCE(S):

MARPAT 142:74445

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) halo(alkyl), (cyclo)alkenyl, (amino)aryl, etc.; X = NH, O or SOm; m =

n = 0-2; p, q = independently 0-5; A = (hetero)aryl; and pharmaceutically acceptable salts, solvates, and physiol. functional derivs. thereof) were prepd. as human papillomaviruses (HPV) inhibitors. For example, II was given in a multi-step synthesis starting from the reaction of 4-chloroaniline with 2-(hydroxymethylene)cyclohexanone. II showed inhibition of HPV 16 with IC50 values of 10 nM in W-12 cellular assay. Thus, I and their pharmaceutical compns. are useful for the treatment or prophylaxis of conditions or disorders due to HPV infection, such as

and cancers (no data). 812649-13-1P, 6-Bromo-N-phenyl-2,3,4,9-tetrahydro-1H-carbazol-1-

812649-14-2P, 6-Bromo-N-phenyl-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine hydrochloride 812649-15-3P, 6-chloro-N-phenyl-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-16-4P, 6-Chloro-N-(4-methoxyphenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-17-5P, 6-chloro-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-19-7P, 6-chloro-N-(4-methylphenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-19-7P, 6-chloro-N-(4-methylphenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-20-P, 6-Bromo-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-22-2P, 6-Bromo-N-(4-fluorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-22-3P, 6-Bromo-N-(4-fluorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-22-4P, 6-Bromo-N-(pyrimidin-2-yyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-22-5P, 6-Chloro-N-(4, 6-dimethoxypyrimidin-2-yyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-26-6P, 8-Chloro-N-(4, 6-dimethoxypyrimidin-2-yyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-26-6P, 8-Chloro-N-(4,

6-Chloro-N-(4-methylpyrimidin-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine 812649-27-7P, 6-Chloro-N-(4,6-dimethylpyrimidin-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine 812649-28-8P, 6-Bromo-N-(pyridin-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-15-3 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

812649-16-4 CAPLUS
1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)(9CI) (CA INDEX NAME)

812649-17-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4-chlorophenyl)-2,3,4,9-tetrahydro-CN (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) hydrochloride 812649-29-99, 6-Bromo-N-(5-propylpyrimidin-2-yl)-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-30-2P, 6-Methyl-N-(pyrimidin-2-yl)-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-31-3P, 6-Methoxy-N-(pyrimidin-2-yl)-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-32-2-4P, N-(4,6-Dimethoxypyrimidin-2-yl)-6-methyl-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine hydrochloride 812649-33-5P, 6-Bromo-N-(4,6-dimethylpyrimidin-2-yl)-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine hydrochloride 812649-34-6P, 6-Bromo-N-(5-(trifluoromethyl)pyrimidin-2-yl)-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-31-6-Bromo-N-(5-(trifluoromethyl)pyrimidin-2-yl)-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-34-6P, (6-Bromo-2, 3, 4, 9-tetrahydro-ll-carbazol-1-yl) aminolnicotinonitrile 812649-34, 9-tetrahydro-ll-carbazol-1-yl) aminolnicotinonitrile 812649-34, 9-tetrahydro-ll-carbazol-1-amine 812649-38-8P, 6-(6-Bromo-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-38-0P, N-Pyrimidin-2-yl-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-39-3P, 6-Methyl-N-(pyrimidin-2-yl)-5, 6, 7, 8, 9, 10-hexahydro-ll-carbazol-1-pyridin-2-yl-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-42-6P, 8-tetrahydro-ll-carbazol-1-amine 812649-42-6P, N-Phenyl-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-43-8P, N-Phenyl-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-43-PP, N-Phenyl-2, 3, 4, 9-tetrahydro-ll-carbazol-1-amine 812649-40-PP, N-Phenyl-2, 3, 4, 9-tetrahydro-ll-carbazo 812649-53-9P, 6-Bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro-1H-carebazole
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of tetrahydrocarbazole derivs. as human papilloma viruses inhibitors)
812649-14-2 CAPUS
1H-Carebazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

812649-18-6 CAPLUS 1H-Carbazol-1-amine, 6-chloro-N-(4-fluorophenyl)-2,3,4,9-tetrahydro-CN (9CI) (CA INDEX NAME)

812649-19-7 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2, 3, 4, 9-tetrahydro-N-(4-methylphenyl)-(CA INDEX NAME)

RN 812649-20-0 CAPLUS

(Continued)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

812649-21-1 CAPLUS 1H-Carbazol-l-amine, 6-bromo-N-(4-chlorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-22-2 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(4-fluorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

812649-23-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyrimidinyl-,
monohydrochloride (9CI) (CA INDEX NAME)

● HCl

812649-24-4 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN L3

812649-25-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4,6-dimethoxy-2-pyrimidinyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-26-6 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methyl-2-pyrimidinyl)- (9C1) (CA INDEX NAME)

812649-27-7 CAPLUS 1H-Carbazol-1-amine, 6-chloro-N-(4,6-dimethyl-2-pyrimidinyl)-2,3,4,9-tetrahydro (9C1) (CA INDEX NAME)

812649-28-8 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyridinyl-, monohydrochloride (9C1) (CA INDEX NAMZ)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

RN 812649-29-9 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2, 3, 4,9-tetahydro-N-(5-propyl-2-pyrimidinyl)-(9CI) (CA INDEX NAME)

812649-30-2 CAPLUS 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

812649-31-3 CAPLUS 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methoxy-N-2-pyrimidinyl- (9CI)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (CA INDEX NAME) (Continued)

RN 812649-32-4 CAPLUS CN 1H-Carbazol-1-amine, N-(4,6-dimethoxy-2-pyrimidiny1)-2,3,4,9-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

812649-33-5 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-{4,6-dimethyl-2-pyrimidinyl}-2,3,4,9-tetrahydro-, monohydrochloride {9CI} (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

• HCl

812649-34-6 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[5-{trifluoromethyl}-2-pyrimidinyl}- (9CI) (CA INDEX NAME)

812649-35-7 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[5-(trifluoromethyl)-2-pyridinyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-36-8 CAPLUS 3-Pyridinecarbonitrile, 6-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)amino]- (9CI) (CA INDEX NAME)

812649-37-9 CAPLUS 1H-Carbazol-lamine, N-2-benzothiazolyl-6-bromo-2, 3, 4, 9-tetrahydro- (9CI) (CA INDEX NAME)

812649-38-0 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-39-1 CAPLUS CN Cyclohept[b]indol-6-amine, 2-bromo-5,6,7,8,9,10-hexahydro-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

812649-41-5 CAPLUS 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyridinyl-, monohydrochloride (9C1) (CA INDEX NAME)

● HCl

812649-42-6 CAPLUS
1H-Carbazole-6-carboxylic acid, 2,3,4,9-tetrahydro-1-(phenylamino)-, methyl ester (9C1) (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

C- OME

RN 812649-43-7 CAPLUS
CN 3-Pyridinecarbonitrile, 6-[(2,3,4,9-tetrahydro-6-methyl-1H-carbazol-1-yl)amino]-, monohydrochloride (9CI) (CA INDEX NAME)

CN N NH H N

• HCl

RN 812649-44-8 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

NHPh H N CF3

● HCl

RN 812649-45-9 CAPLUS
CN 1H-Carbazol-l-amine, 2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

RN 812649-49-3 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(2-methoxyphenyl)-(9CI) (CA INDEX NAME)

RN 812649-50-6 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-N-(2-chlorophenyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

C1 NH H H

RN 812649-51-7 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(2-fluorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA TNDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NHPh H

RN 812649-46-0 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(3-methoxyphenyl)(9CI)
(CA INDEX NAME)

RN 812649-47-1 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-N-(3-fluoropheny1)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

F NH B

RN 812649-48-2 CAPLUS CN 1H-Carbarol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-1H-indo1-5-yl- (9CI) (CA INDEX NAME)

L3 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continue

F NH H

RN 812649-52-8 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(3,4-dichlorophenyl)-2,3,4,9-tetrahydro(9C1) (CA INDEX NAME)

RN 812649-53-9 CAPLUS
CN 1H-Carbazole, 6-bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

, H

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMA

3 ANSWER 12 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN CCESSION NUMBER: 2003:726528 CAPLUS

ACCESSION NUMBER:

2003:726528 CAPLUS

2004:726528 CAPLUS

139:371731

Photophysical Properties of Directly Linked Linear

Porphyrin Arrays

AUTHOR(S):

CORPORATE SOURCE:

National Creative Research Initiatives Center for

Ultrafast Optical Characteristics Control and

Department of Chemistry, Yonsei University, Seoul,

120-749, S. Korea

Journal of Physical Chemistry A (2003), 107(42),

3791-8816

CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER:

American Chemical Society

DOUMENT TYPE:

JOURNAL TYPE:

JOURNAL ARRAYS CONNECTED BY A VIEWPOINT OF CHEMISTRY AND ARRAYS CONNECTED BY A VIEWPOINT OF CHEMISTRY AND ARRAYS SOURCE Inquise and electronics. From a viewpoint of operational requirements, the porphyrin arrays should have the very regular plagment arrangements which allow a facile light energy or charge flow along the arrays but do not result in the alteration of individual properties of the constituent pigments leading to formation of so-called energy or charge sink. In these respects, the directly compled (orthogonal and fused) porphyrin arrays without any linkers are ideal, because the conformational heterogeneity mainly arising from a diehedral angle distribution between the neighboring porphyrin moieties should be minimized. In addition, the electronic of the linker can be disregarded in design strategy of mol. photonic devices, because the linker can also be considered as a transmission element in electronic communication. Considering these features, these types (orthogonal vs fused) of porphyrin arrays would be one of the most suitable synthetic mol. modules for the realization of mol. photonic and electronic devices. To unveil the functionalities of various porphyrin arrays, starting from the dihedral angle dependence on the photophys. properties of the pophyrin arrays with ample electronic interactions will be promising in the applications such as mol. wires, sensors, optical nonlinear materials, and so on.

17 48645-26-5

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PPP (Physical)

(Physical process); PROC (Process)
(photophys. properties of directly linked linear porphyrin arrays)
486445-26-5 CAPLUS
Poly[5,15-bis[4-(1,1-dimethyltridecyl)phenyl]-21H,23H-porphine2,20,18:8,10,12-hexayl-xN21,xN22,xN23,xN24] zinc
complex] (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

PAGE 1-A

PAGE 1-B

REFERENCE COUNT:

THERE ARE 121 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE FORMAT

L3 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2003:726516 CAPLUS DOCUMENT NUMBER: 139:338148

TITLE:

An o-Iminothioquinone: Its Cycloaddition To Produce

Indologlycoside and Its Self-Dimerization To Form a Dithio-Diazocycloctane, the Structure Assignment of Which Is Based on the DFT Prediction of Its IR

Spectrum

Spectrum
Diep, Vinh; Dannenberg, J. J.; Franck, Richard W.
Department of Chemistry, Hunter College, CUNY, New
York, NY, 10021, USA
Journal of Organic Chemistry (2003), 68(20), AUTHOR(S): CORPORATE SOURCE:

SOURCE: 7907-7910 CODEN: JOCEAH; ISSN: 0022-3263 American Chemical Society

PUBLISHER: Journal

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S):

UNGE: English R SOURCE(S): CASREACT 139:338148 An unusual heterodiene, an indolothiono quinone, undergoes cycloaddn. with

a glycal to form an indole-N-glycoside. A novel dimer of the indolothionoquinone is assigned its structure on the basis of a match between its predicted and observed IR spectrum.

616883-32-0P

RI: PBP [Oran-1-1-1]

,883-32-09 : PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and structural characterization of an indologlycoside and its

dimerization a dithio-diazocycloctane)
616883-32-0 CAPLUS
1H-Isolndole-1,3(2H)-dione, 2-(9H-carbazol-1-ylthio)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L3 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2002:870385 CAPLUS DOCUMENT NUMBER: 138:114936 Photophysical properties of poth Cho, Hyun Sun; Jeong, Dae Hong.

Seoul,

138:114936
Photophysical properties of porphyrin tapes
Cho, Hyun Sun; Jeong, Dae Hong; Cho, Sung; Kim,
Dongho; Matsuzaki, Yoichi; Tanaka, Kazuyoshi; Tsuda,
Akihiko; Osuka, Atsuhiro
Center for Ultrafast Optical Characteristics Control
and Department of Chemistry, Yonsei University,

CORPORATE SOURCE:

SOURCE:

120-749, S. Korea Journal of the American Chemical Society (2002), 124(49), 14642-14654 CODEN: JACAST; ISSN: 0002-7863 American Chemical Society

PUBLISHER:

Journal English

DOCUMENT TYPE: LANGUAGE: AB The novel MAGE: English The novel fused Σ (Elijosphyrin arrays (Tn, porphyrin tapes) in which the porphyrin macrocycles are triply linked at meso-meso, β - β , β - β positions have been investigated by steady-state and time-resolved spectroscopic measurements along with theor. MO calcus.

absorption spectra of the porphyrin tapes show a systematic downshift to the IR region as the number of porphyrin pigments increases in the

arrays.

The fused porphyrin arrays exhibit a rapid formation of the lowest

states (for T2, .apprx.500 fs) via fast internal conversion processes

upon photoexcitation at 400 nm (Soret bands), which is much faster than the internal conversion process of .apprx.1.2 ps observed for a monomeric

f) porphyrin. The relaxation dynamics of the lowest excited states of the porphyrin tapes were accelerated from .apprx.4.5 ps for the T2 dimer to .apprx.0.3 ps for the T6 hexamer as the number of porphyrin units

increases,
being explained well by the energy gap law. The overall photophys.
properties of the porphyrin tapes were observed to be in a sharp
contrast to
those of the orthogonal porphyrin arrays. The PPP-SCI calculated
charge-transfer probability indicates that the lowest excited state of

the porphyrin tapes (Tn) resembles a Wannier-type exciton closely, whereas the

lowest excited state of the directly linked porphyrin arrays can be considered as a Frenkel-type exciton. Conclusively, these unique photophys. properties of the porphyrin tapes have aroused much interest

in the fundamental photophysics of large flat organic mols. as well as in

the possible applications as elec. wires, IR sensors, and nonlinear optical materials. 486445-26-5 RL: PEP (Physical, engineering or chemical process); PRP (Properties); ΙT

(Physical process); PROC (Process)
(photophys. properties of fused zinc porphyrin studied by
Steady-stateand time-resolved spectroscopy and theor. MO calcns.)
RN 48545-26-5 CAPLUS

- ANSWER 14 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Poly[[5,15-bis|4-(1,1-dimethyltridecyl)phenyl]-21H,23H-porphine-2,20,18:8,10,12-hexyl-kx21,kx22,kx23,kx24] zinc complex] (9CI) (CA INDEX NAME)
- ANSWER 14 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN · (Continued)

PAGE 1-A

PAGE 1-B

REFERENCE COUNT:

THERE ARE 55 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

SOURCE:

L3 ANSWER 15 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:436241 CAPLUS
DOCUMENT NUMBER: 135:195514
TITLE: Transformation of 5H,1H-indolo[3,2-b]carbazole through 5,11-didehydroindolo[3,2-b]carbazole through 5,11-didehydroindolo[3,2-b]carbazole yudina, L. N.; Preobrazhenskaya, M. N.; Korolev, A.

M. CORPORATE SOURCE:

G. F. Gauze Research Institute for the Search of New Antibiotics, Russian Academy of Medical Sciences, Moscow, 119867, Russia Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2001), Volume Date 2000, 36(3), 1112-1113 CODEN: CHCCAL: ISSN: 0009-3122 Consultants Bureau Journal English CASREACT 135:195514

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE(S):

III

Treatment of 5H,11H-indolo[3,2-b]carbazole (I) with DDQ gave 5,11-didehydroindolo[3,2-b]carbazole (II), which reacted with DDHQ to give

give
III.
356039-99-1P
RL: SFN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 356039-99-1 CAPLUS
CN Benzenecarboximidic acid,
3,4-dichloro-6-cyano-5-[(5,11-dihydroindolo[3,2-b]carbazol-6-yl)oxy]-2-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L3 ANSWER 16 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER:

DOCUMENT NUMBER:

130:305998

In vitro metabolism of a new anticancer agent,
6-N-formylamino-12,13-dihydro-1,11-dihydroxy-13(B-D-qlucopyranoxyl)5H-inddol (2,3-A)pyrrclo
(3,4-Clcarbazole-5,7(6H)-dione (NB-506), in mice,
rats, dogs, and humans

AUTHOR(S):

Takenaga, N.; Haseggawa, T.; Ishii, M.; Ishizaki, H.;
Hata, S.; Kamei, T.

CORPORATE SOURCE:

Drug Metabolism, Development Research Laboratories,
Banyu Pharmaceutical Co., Ltd., Saitama, 360-0214,
Japan

SOURCE:

Drug Metabolism and Disposition (1999), 27(2),

PUBLISHER: American Society for Pharmacology and Experimental
PUBLISHER: American Society for Pharmacology and Experimental
AMEDIAGE: American Society for Pharmacology and Experimental
AMEDIAGE: Boglish
Bournal
LANGUAGE: Boglish
Boglish of 6-N-formylamino-12,13-dihydro-1,11-dihydroxy-13-(B-Dglucopyranosyl)5H-indolo [2,3-a]pyrrolo [3,4-c]carbazole-5,7(6H)-dione
(NB-506), a potent inhibitor of DNA topoisomerase I, was characterized in
mice, rats, dogs, and humans in vitro. NB-506 was deformylated to ED-501
in mouse and rat plasma with enzyme activity of 140 and 116 pmol/min/mg
protein, resp. The enzyme activity in dog and human plasma was found to
be less than 1.7 pmol/min/mg protein. In liver 59 and small intestine S
samples from mice and rats, activity of the enzyme was very low. Also,
there was no activity in the liver or small intestine of dogs and humans.
The enzyme involved in the conversion of NB-506 to ED-501 in rat plasma

a rodent-specific serine enzyme with a mol. mass of 138KDa. The Vmax a Km values were 6.3 nmol/min/mL plasma and 54 µM at an optimum pH of 7.4, resp. Although NB-506 was converted to ED-551 in dog and human plasma in vitro, no conversion was observed in mouse and rat plasma. human plasma this conversion was not affected by heat treatment (100°C for 1 min), but was inhibited completely by 50 mM EDTA, indicating that the reaction is a chemical reaction catalyzed by metal

Although NB-506 was not metabolized by cytochrome P 450 isoenzymes in liver, this drug was glucuronized in mice, rats, and humans, but not in dogs. These results suggest that a species difference in the metabolism

NB-506 occurred in the liver as well as in plasma. There appeared to be species differences in the metabolism of NB-506 in vitro, correlating

with the species-dependent pharmacokinetics of this drug in vivo.
217187-87-6, ED 594
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(in vitro metabolism of a new anticancer agent, NB-506, in mice, rats, dogs, and humans)
217187-87-6 CAPLUS
β-D-Glucopyranosiduronic acid, 6-(formylamino)-12-β-D-glucopyranosyl-6,7,12,13-tetrahydro-11-hydroxy-5,7-dioxo-5H-indolo(2,3-

ANSWER 16 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN a)pyrrolo[3,4-c]carbazol-1-yl (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

CQ2H

REFERENCE COUNT:

FORMAT

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L3 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1999:172499 CAPLUS DOCUMENT NUMBER: 130:305997 TITLE: In vivo personal control of the control of the

130:305997
In vivo metabolism of a new anticancer agent,
6-N-formylamino-12,13-dihydro-1, 11-dihydroxy-13(β-D-glucopyranosil) 5H-indolo [2,3-A]pyrrolo
[3,4-C]carbazole-5, 7(6H)-dinon (NB-506) in rats and
dogs: pharmacokinetics, isolation, identification,

and AUTHOR (S):

quantification of metabolites
Takenaga, N.; Ishii, M.; Nakajima, S.; Hasegawa, T.;
Iwasa, R.; Ishizaki, H.; Kamei, T.
Drug Metabolism, Development Research Laboratories,
Banyu Pharmaceutical Co., Ltd., Saitama, 360-0214,

CORPORATE SOURCE:

Japan Drug Metabolism and Disposition (1999), 27(2),

SOURCE: 205-212

205-212

CODEN: DNDSAI/ ISSN: 0090-9556

American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: Anglish Grant Society for Pharmacology and Experimental Therapeutics
Glucopyranosil/5H-indolo [2,3-a]pyrrolo [3,4-c]carbazole-5,7(6H)-dione (NB-506), a potent inhibitor of DNA topoisomerase I, is currently under development for the treatment of cancer. We investigated the pharmacokinetics of NB-506 after i.v. administration in rats and dogs.
The plasma concentration of NB-506 decreased biexponentially in rats and dogs

with terminal half-lives of approx. 2 h. The area under the curve increased nonlinearly with increasing dose in rats. In contrast, there was a linear relationship between the area under the curve and the dose

in dogs. In rats, the plasma clearance decreased with increasing dose up to 187.5 mg/m2 but remained virtually unchanged at the highest dose. The Vdss of NB-506 in rats and dogs was much greater than the plasma volume, indicating that NB-506 is highly distributed to tissue from plasma in these animals. There were marked species differences in the plasma conons. of ED-501 after i.v. administration of NB-506 to rats and dogs. To better understand the mechanisms of nonlinear pharmacokinetics in

in vivo metabolites were determined After i.v. administration of [14C]NB-506

]NB-506
to rats, two unknown metabolites (RBM-1 and RBM-2), deformyl metabolite (ED-501), and unchanged drug (NB-506) were identified. Mass and NNR spectra anal. revealed that RBM-1 is an 11-0-glucuronide of NB-506 (ED-594) and that RBM-2 is an 11-0-glucuronide of ED-501 (ED-595). In this study, the pharmacokinetics of NB-506 was demonstrated to be nonlinear in rats, probably because of saturation of the enzyme systems catalyzing the deformylation and glucuronidation of NB-506 in rats. 217187-87-6, ED 594 217188-819, ED 595
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

RN CN

(Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(in vivo metabolism of a new anticancer agent NB-506 in rats and dogs)
217167-67-6 CAPLUS
β-D-Glucopyranosiduronic acid, 6-(formylamino)-12-β-Dglucopyranosiduronic acid, 6-(formylamino)-12-β-Dglucopyranosy1-67,712,13-tetrahydro-11-hydroxy-5,7-dioxo-5H-indolo[2,3-a)pyrrolo[3,4-c]carbazol-1-yl (9CI) (CA INDEX NAME)

L3 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Absolute stereochemistry.

217188-11-9 CAPLUS β-D-Glucopyranosiduronic acid, 6-amino-12-β-D-glucopyranosyl-6,7,12,13-tetrahydro-11-hydroxy-5,7-dioxo-5H-indolo[2,3-a]pyrrolo[3,4-c|carbazol-1-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry

REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

Searched by Jason M. Nolan, Ph.D.

L3 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) L3 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:667211 CAPLUS
DOCUMENT NUMBER: 130:22652
TITLE: Metabolism of carvediol in dogs, rats, and mice
AUTHOR(S): Schaefer, William H.: Politowski, James; Hwang,
Bruce; Divon Frank, Jr.: Goalvin, Anne; Gutzait, Louis:

TITLE:

AUTHOR(S):

Bruce;

Dixon, Frank, Jr.: Goalwin, Anner Gutzait, Louis:
Anderson, Kathleen: Debrosse, Charles; Bean, Mark:
Rhodes, Gerald R.

CORPORATE SOURCE:

Departments of Drug Metabolism and Pharmacokinetics,
SmithKline Beecham Pharmaceuticals, USA

Drug Metabolism and Disposition (1998), 26(10),
358-969

CODEN: DNDSAI: ISSN: 0090-9556

PUBLISHER:

Williams & Wilkins

DOCUMENT TYPE:
Journal
LANGUAGE:
English
AB The excretion and biotransformation of carvedilol
[1-[carbacoly]-(4)-oxy]3-[(2-methoxyphenoxyethyl) amino]-2-propanol], a new, multiple-action,
neurohormonal antagonist that exhibits the combined pharmacol. activities
of p-adrenoreceptor antagonism, wasodilation, and antioxidin, were
investigated in dogs, rats, and mice. Carvedilol was absorbed well, and
biliary secretion was predominant in each species. Carvedilol was
metabolized extensively in each species, and elimination of unchanged
compound was minor in bile duct-catheterized rats and dogs. In dogs,
glucuronidation of the parent compound and hydroxylation of the
carbazolyl

ring, with subsequent glucuronidation, were the major metabolite were
formed by hydroxylation of the carbazolyl ring, with subsequent
glucuronidation. Mice displayed the most complicated metabolite profile;
glucuronidation of the parent compound and hydroxylation of eight experiments
represented by the parent compound and hydroxylation of the carbazolyl ring, with subsequent
glucuronidation of the parent compound and hydroxylation of the carbazolyl ring, with subsequent
glucuronidation of the parent compound and hydroxylation of the carbazolyl ring, with subsequent
glucuronidation of the parent compound and hydroxylation of ethe carbazolyl ring, with subsequent
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glucuronidation of the parent compound and hydroxylation of ethe carbazolyl ring, with subsequent
glucuronidation of the parent compound and hydroxylation of ethe carbazolyl ring, with subsequent
glucuronidation

L3 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

Absolute stereochemistry.

L3 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

131087-99-5 CAPLUS methoxyphenoxylethyl]amino]propoxyl-9H-carbazol-1-yl (9CI) (CA INDEX

Absolute stereochemistry.

REFERENCE COUNT: THIS

FORMAT

THERE ARE 34 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

L3 ANSWER 19 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1998:612719 CAPLUS DOCUMENT NUMBER: 130:47074

DOCUMENT NUMBER:

TITLE:

Studies on the displosion of [14C]NB-506: plasma concentration-time profile, distribution, metabolism and excretion of [14C]NB-506 after single and

and excretion of [14C)NB-506 after single and intravenous administration in rats

AUTHOR(S): Ishii Mikklo, Takenaga, Norihiror Ishizaki, Hiroyuki; Kamel, Toshio, Ninomiya, Shin-ichi; Esumi, Yoshio Development Research Laboratorics, Banyu Pharmaceutical Co., Ltd., Saitama, 360-0214, Japan SOURCE: Yakubutau Dotai (1998), 13(4), 337-345

FUBLISHER: Nippon Yakubutau Dotai Gakkai Journal Jour

and kidney, and then decreased and were lower than 10% of maximum radioactivity at 72 h. 3. Within 120 h after a single i.v. nistration of [14C]NB-506 to male rats, 9.8 and 88.3% of dose were excreted into urine and feces, resp. Biliary excretion was 82.9% in male rats. The enterohepatic circulation of [14C]NB-506 was not observed in male rats.

excretion of radioactivity in female rats was similar to that in male rats. 4. After a single i.v. administration of (14C)NB-506 to male rats 40.0, 23.8, 6.3 and 1.51 of dose were excreted to bile (0-6 h) as intact NB-506, NB-506 glucuronide (ED-594), NB-506 deformy1 form (ED-501) and ED-501 glucuronide (ED-595), resp. The 6.21 of administered dose in

(0-4 h) corresponded to intact NB-506 and 0.7% of dose was excreted to urine as ED-594 and ED-501. 5. The plasma levels of radioactivity at 5 min, 4, 24 h after the 5th dosing were higher than those after the first dosing. Moreover, the levels of $AUC(0-\omega)$ and $11/2\gamma$ of the 5th dosing were 2.1 and 2.3 times higher than those of the first dosing,

resp.

These results indicate that {14C]NB-506 tend to accumulate in plasma

the multiple dosing. The accumulation ratio was calculated based on the plasma levels of radioactivity at 24 h after the first and the 5th

dosing: this value was 3.85. On the other hand, the accumulation factor, which

ANSWER 19 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) was estd. from the elimination rate const., was calcd. to be 3.56. Therefore, the accumulation ratio was almost of the same value as the predicted accumulation factor. These results suggest that it is possible to predict the disposition of [14C]NB-506 after the multiple dosing and the possibility that the crucial accumulation of [14C]NB-506 may arise from the multiple dosing is low. 6. No change in the daily excretion of radioactivity in urine and feces was obsd. during 5-day repeated administration. Within 168 h after the last dosing, urinary and fecal excretion of radioactivity were 7.5 and 90.18 of dose, resp., indicating that the main elimination route is fecal excretion.
21/187-87-6, ED 594 21/198-11-9, ED 55
RL: BPR (Biological process); RSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(studies on the displosion of [14C]NB-506: plasma concentration-time

ile,
distribution, metabolism and excretion of [14C]NB-506 after single and repeated i.v. administration in rata)
27187-87-6 CAPLUS
β-D-Glucopyranosiduronic acid, 6-(formylamino)-12-β-D-glucopyranosy1-67, 12,13-tetrahydro-11-hydroxy-5,7-dioxo-5H-indolo[2,3-a]pyrrolo[3,4-c]carbazol-1-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

217188-11-9 CAPLUS
β-D-Glucopyranosiduronic acid, 6-amino-12-β-D-glucopyranosyl6,7,12,13-tetrahydro-11-hydroxy-5,7-dioxo-5H-indolo[2,3-a]pyrrolo[3,4-c]carbazol-1-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 20 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
1995:686731 CAPLUS
123:113989
Stabilization of polyethylene against thermal oxidation
Oxidation
Daszkiewicz, Zdzislaw; Sudol, Marek; Kyziol, Janusz
B.: Nowakowska, Maria
PATENT ASSIGNEE(S):
Wysza Szkola Pedagogiczna im. Powstancow Slaskich, Pol.
Pol., 6 pp.
CODEN: POXXA7
DOCUMENT TYPE:
LANGUAGE:
PAHLUY ACC. NUM. COUNT: 1
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PL 159744 PRIORITY APPLN. INFO.:	В1	19930129	PL 1989-282691 PL 1989-282691	19891207 19891207

OTHER SOURCE(S): MARPAT 123:113989

Carbazole derivs. I [R = H, Et, or PhCH2, Rl = 1- or 3-(2-naphthylamino)] are useful for the title process at 0.05-0.5% concentration 195934-75-9, 1-(2-Naphthylamino)carbazole Rl: MOA (Modifier or additive use); USES (Uses) (naphthylaminocarbazole derivs. as antioxidants for polyethylene) 195934-75-9 CAPLUS (Modifier or additive use); USES (Uses) (CA INDEX NAME)

L3 ANSWER 21 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:240048 CAPLUS
100CUMENT NUMBER: 122:31324
Method for preparation of new naphthyl derivatives of aminocarbazoles useful as polymer stabilizers
Daszkiewicz, Zdzialew, Sudol, Marcek Kyziol, Janusz Wyzeza Szkola Pedagogiczna im. Powstancow Slaskich, Pol.
SOURCE: Pol., 4 pp.
CODEN: POXXAT
DOCUMENT TYPE: PATEMI INFORMATION: POLIS
FAMILU ACC. NUM. COUNT: 1
PATEMI INFORMATION: POLIS

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. APPLICATION NO. DATE KIND DATE PL 1989-278902 PL 1989-278902 PL 159916 PRIORITY APPLN. INFO.: В1 19930129 19890414

OTHER SOURCE(S):

MARPAT 122:31324

Title compds. I $\{R=H, alkyl, CH2Ph\}$ and II, useful as antioxidants and heat stabilizers for olefinic polymers (no data), are prepared by fusion AB

of corresponding 3-amino-9-R-substituted carbazoles or 1-aminocarbazole with a 5- to 15-fold molar excess of 2-naphthol. For example, 0.1 mol 3-amino-9-ethylcarbazole was dissolved in 1 mol molten 2-naphthol, and

the mixture was kept at 410 K for 24 h with subsurface bubbling of N2. After addition of 0.1 L DMF to decrease viscosity, the mixture was poured into

solution of 80 g NaOH in 0.8 L H2O, and the precipitate was filtered,

washed, and dissolved in 1:1 THF-toluene. After washing with base and acid to remove

L3 ANSWER 22 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1992:469729 CAPLUS DOCUMENT NUMBER: 117:69729

Substituted 1,2,3,4-tetrahydrocyclopent[b]indoles, 1,2,3,3a,4,8a-hexahydrocyclopent[b]indoles and TITLE:

related

INVENTOR (S):

compounds
Ong, Helen H.; O'Malley, Gerard J.; Merriman, Michael
C.; Palermo, Mark G.
Hoechst-Roussel Pharmaceuticals Inc., USA
U.S., 22 pp.
CODEN: USXXAM PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE US 5100891 US 5192789 RO 112505 FI 9200192 FI 102174 PL 167465 PL 169417 CZ 282732 CA 2059610 CA 2059610 NO 9200235 US 1991-642952 US 1992-818703 RO 1992-149168 FI 1992-192 19910118 19920109 19920115 19920116 19920331 A A B1 19930309 19971030 A B B1 19920719 19981030 19981030 19950930 19960731 19970917 PL 1992-296651 PL 1992-293209 CZ 1992-129 CA 1992-2059610 B1 B6 A1 C A B C A B2 19920116 19920116 19920117 19920719 20020402 19920720 19951211 NO 9200235 NO 178397 NO 178397 AU 9210279 NO 1992-235 19920117 19960320 AU 1992-10279 19920117 19920723 19940616 19920930 19921120 19950130 19970420 19920729 19971001 AU 9210279 AU 650315 ZA 9200341 JP 04334367 HU 67027 ZA 1992-341 JP 1992-6681 HU 1992-172 RU 1992-5010763 EP 1992-100816 19920117 A A A2 C1 19920117 19920117 RU 2077530 19920117 19920118 EP 496314 EP 496314 GB, GR, TT, LI, LU, NL, PT, AT 1992-100816 1: ES 1992-100816 1: BR 1992-171 1: US 1992-976067 1: US 1994-177035 1: US 1995-472586 1: US 1997-396 1: US 1997-ES, FR, 19971015 7, SE 19920118 19920118 19920121 19921113 19940104 19950607 19970130 19980201 19921006 19940329 19940329 19951205 19960507 19970130 20010615 19970130 20010330 FI 1997-397 19970130 FI 2000-1775 20000810 20000810 20011031 FI 107919 PRIORITY APPLN. INFO.: US 1991-642952 A2 19910118 us 1992-818703 A3 19920109

FI 1992-192

ANSWER 22 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN US 1992-976067 (Continued) A3 19921113

US 1994-177035

A3 19940104

OTHER SOURCE(S): CASREACT 117:69729; MARPAT 117:69729

Title compds. I [n = 2, 3, 4, 5; X = H, lower alkyl, lower alkoxy, OH, halo, CF3, NO2; Rl = H, lower alkyl, lower alkenyl, lower alkynyl, amino lower alkyl, cycloalkyl, cycloalkenyl, aryl, pyrrolidinoalkyl, plperidinoalkyl, morpholinoalkyl, etc.; R2 = H, lower alkyl, formyl,

alkylcarbonyl, benzyloxycarbonyl, etc.; NR1R2 = pyrrolidino, piperidino, morpholino, piperazino, etc.; R3 = H, lower alkyl, aryl lower alkyl,

alkylcarbonyl, lower alkoxycarbonyl; R4 = O2CNR5R6 (R5 = lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, aryl, etc.; R6 = H, lower

aryl, aryl lower alkyl; NR5R6 = pyrrolidino, piperidino, morpholino, piperazino, etc.]] were prepared as agents for alleviating various memory dysfunctions characterized by a cholinergic deficit such as Alzheimer's disease. Thus, 1,2-dhydrocyclopent(b)indoi-3(2H)-one II (R7 = H) was acylated with ClCH2COCl in the presence of ALCl3 in CH2Cl2 to give II (R7 = ClCH2CO), which was oxidized with m-chloroperbenzoic in the presence of Na phosphate in CHCl3 to give II (R7 = ClCH2CO2). The latter was treated with cyclopropylamine in the presence of TiCl4 in toluene to give the imine III, which was reduced with NaBH4 in Me2CHOH/MeOH (5:1) to give the amine IV (R8 = H), which was treated with Me isocyanate in the presence

1,8-diazabicyco[5.4.0]undec-7-ene in CH2Cl2 to give IV (R8 = MeNHCO) (V). V at 3.5 µM inhibited brain acetylcholinesterase by 50%; V also inhibited monoaulne oxidases. 142283-79-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 142283-79-2 CAPLUS Cyclopent(b)indol-3-amine, N-cyclopropyl-1,2,3,4-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

IT

A 19920116

A 19901025

(Continued) ANSWER 22 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

• HC1

L3 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:679992 CAPLUS

105:279992 Preparation and formulation of carbazole-3,4dicarboximides and analogs as antitumor agents

Nagai, Takashi; Myokan, Isao; Keishi, Funaki; Ohta,
Kenji: Taya, Nobuhisa: Miyabata, Shinji; Shibata,
Masaaki; Mikami, Hidetada; Hori, Takako

Toyama Chemical Co., Ltd., Japan

Ger. Offen., 98 pp.

CODEN: GWXXEX

PATENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
DE 4034687	A1	19910502	DE 1990-4034687	19901031		
DE 4034687	C2	19991202				
JP 04178387	A	19920625	JP 1990-288069	19901025		
JP 3027599	B2	20000404				
US 5166204	A	19921124	US 1990-605430	19901030		
CA 2028960	A1	19910502	CA 1990-2028960	19901031		
CA 2028960	С	19990119				
DK 9002618	A	19910502	DK 1990-2618	19901031		
NL 9002366	A	19910603	NL 1990-2366	19901031		
FR 2655345	A1	19910607	FR 1990-13552	19901031		
GB 2239013	A	19910619	GB 1990-23568	19901031		
GB 2239013	В	19930602				
SE 9003476	A	19920501	SE 1990-3476	19901031		
SE 509700	C2	19990222				
BE 1004069	A3	19920915	BE 1990-1032	19901031		
CH 682151	A5	19930730	CH 1990~3464	19901031		
PRIORITY APPLN. INFO.:			JP 1989-285548 A	19891101		
			JP 1990-205443 A	19900802		

JP 1990-288069

OTHER SOURCE(S):

MARPAT 115:279992

$$R^{1}$$
 R^{1}
 R^{2}
 R^{3}
 R^{3}
 R^{3}
 R^{3}

- ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
- AB The title compds. [I; G = O, Son, NR2; Rl, R3 = H, halo, NO2, OH, (un)substituted alkyl, aryl, etc.; R2 = (un)substituted (ar)alkyl, aryl, CONIZ, acyl; R6R7 = CON(Y2)CO; Y = bond, alkylene; Z = halo, (un)protected
 OH, NR4R5, etc.; R4,R5 = H, (un)substituted (cyclo)alkyl, aralkyl, acyl, aryl; NR4R5 = (un)substituted heterocyclyl; n = 0-2) were prepared Thus, N-benzyl-4-oxocyclohexane-1,2-dicarboximide was cyclocondensed with PhNNNRA and 1 of the isomeric products aromatized with DOQ to give title compound II (R = CH2Ph, R1 = R3 = H) which was converted in 2 steps to II (R
- CH2CH2NMe2) (III; R1 = R3 = H). III (R1 = OH, R3 = Me) gave life extension of >377% that of controls in mice with i.p. L-121- ascites
- cells at 1 mg/kg i.p.
 135555-15-6P 135555-21-4P 135555-52-1P
 135555-53-2P
 135555-53-2P
 13555-53-2P
 (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, in preparation of antitumor agents)
 135555-15-6 CAPLUS
 9H-Carbazole-3, 4-dicarboxylic acid, 6-methoxy-1-phenoxy-, dimethyl ester
 (9CI) (CA INDEX NAME)

135555-21-4 CAPLUS 1H-Furo[3,4-c]carbazole-1,3(6H)-dione, 9-methoxy-5-phenoxy- (9CI) (CA INDEX NAME)

135555-52-1 CAPLUS
9H-Carbazole-3,4-dicarboxylic acid,
i-methoxyphenoxy)-6-(phenylmethoxy), dimethyl ester (9CI) (CA INDEX NAME)

ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) о- сн₂- Ph

135555-53-2 CAPLUS
1H-Furo[3,4-c]carbazole-1,3(6H)-dione, 5-(4-methoxyphenoxy)-9(phenylmethoxy)- (9CI) (CA INDEX NAME)

135551-87-0P 135551-88-1P 135552-28-2P 135552-29-3P 135553-08-1P 135553-09-2P 135553-16-1P 135553-17-2P 135553-18-3P 13553-19-4P 135553-24-1P 135553-25-2P RL: BRC (Biological activity or effector, except adverse); BSU IT

(Biological logical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOD, (Biological study); PREP (Preparation); USES (Uses) (preparation of, as antitumor agent) 135551-87-0 CAPLUS Pyrrolo[3,4-c]carbarole-1,3(2H,6H)-dione, 2-[2-(dimethylamino)ethyl]-9-methoxy-5-phenoxy- (9CI) (CA INDEX NAME)

L3 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 135551-88-1 CAPLUS
CN Pycrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-{2-(dimethylamino)ethyl}-9-methoxy-5-phenoxy-, hydrochloride (9CI) (CA INDEX NAME)

Ox HC1

RN 135552-28-2 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-[2-(dimethylamino)ethyl]-9hydroxy-5-phenoxy- (9CI) (CA INDEX NAME)

RN 13555-29-3 CAPLUS
CN Pyrrolof3,4-c[carbazole-1,3(2H,6H)-dione, 2-[2-(dimethylamino)ethyl]-9hydroxy-5-phenoxy-, hydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 135553-16-1 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-[2-(dimethylamino)ethyl]-9hydroxy-5-(4-hydroxyphenoxy)- (9CT) (CA INDEX NAME)

RN 135553-17-2 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-[2-(dimethylamino)ethyl]-9hydroxyy-5-(4-hydroxyphenoxy)-, monohydrochloride (SCI) (CA INDEX NAME)

• HC1

RN 135553-18-3 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-[2-(diethylamino)ethyl]-9-hydroxy-5-phenoxy- (9CI) (CA INDEX NAME)

L3 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

•x HCl

RN 135553-08-1 CAPLUS
CN Pyrcolo[3,4-c]cacbazole-1,3(2H,6H)-dione, 2-[2-(diethylamino)ethyl]-9-methoxy-5-phenoyy- (9CI) (CA INDEX NAME)

RN 135553-09-2 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione,
2-(2-(dimethylamino)ethyl]-5-(4methoxyphenoxy)-9-(phenylmethoxy)- (9CI) (CA INDEX NAME)

L3 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 135553-19-4 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-(2-(diethylamino)ethyl]-9hydroxy-5-phenoxy-, monohydrochloride (SCI) (CA INDEX NAME)

• HCl

RN 135553-24-1 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-[2-(dimethylamino)ethyl]-9-hydroxy-5-(4-methoxyphenoxy)- (5CI) (CA INDEX NAME)

RN 13555-25-2 CAPLUS
CN Pyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione, 2-(2-(dimethylamino)ethyl)-9hydroxy-5-(4-methoxyphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 23 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L3 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

136657-38-0 CAPLUS B-D-Glucopyranosiduronic acid, 4-[2-hydroxy-3-[[2-(2-methoxyphenoxy]ethyl]amino]propoxy]-9H-carbazol-1-yl, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

136657-39-1 CAPLUS
B-D-Glucopyranosiduronic acid, 5-[2-hydroxy-3-[[2-[2-methoxyphenoxy]+thyl]amino]propoxy]-9H-carbazol-1-yl, (R)- (9CI) (CA INDEX NAME)

ACCESSION NUMBER:
1991:574019 CAPLUS
115:174019 CAPLUS
115:174019
115:174019 CAPLUS

Two enantiomerically radiolabeled carvedilol pseudoracemates, 14C-labeled R(+)/unlabeled S(-)-carvedilol and 14C-labeled S(-)/unlabeled R(+)-carvedilol, were reconstituted and administered orally and i.v. to sep. groups of bile duct-cannulated rats to determine the biliary excretion of

excretion of
carvedilol enantiomers and the stereochem. composition of metabolites
excreted
into the bile. Oral administration of these pseudoracemates produced no
enantiomeric difference in the biliary excretion of the radioactivity
derived from the enantiomers, whereas i.v. administration did result in

enantiomeric difference: the biliary excretion rate of the radioactivity derived from R(+)-enantiomer was higher than that from S(-)-enantiomer. After administration by the two routes, two carbazole ring-hydroxylated glucuronides, 1-hydroxycarvedilol O-glucuronide (1-ONCG) and 8-hydroxycarvedilol O-glucuronide (8-OHCG), were detected as the major metabolites in the bile. The S/R enantiomer ratios of 1-OHCG were 0.59 for oral dosing and 0.43 for i.v. dosing, suggesting that the formation

for oral dosing and 0.43 for i.v. dosing, suggesting that the formation of 1-OHCG is selective for R(+)-enantiomer, while the S/R ratios of 8-OHCG showed values of 3.29 and 2.63 for oral and i.v. administrations, resp., favoring S(-)-enantiomer. Since corresponding hydroxylated metabolites are rapidly biotransformed to glucuronides that are excreted predominantly in the bile, the stereoselectivity of these glucuronides presumably reflects that of carbazole ring hydroxylation.

1 13657-37-9 136557-38-0 136557-39-1 136557-39-1 136557-30-4
RL: FORM (Formation, nonpreparative) [formation of, as carvedilol metabolite, after oral and i.v. administration of racemate, stereoselectivity in)

RN 13657-37-9 CAPLUS
CN P-D-Glucopyranosiduronic acid, 4-(2-hydroxy-3-[[2-(2-methoxyphenoxy)-thyl]amino]propoxy]-9H-carbazol-1-yl, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN Absolute stereochemistry. (Continued)

136657-40-4 CAPLUS 13657-40-4 CAPONS
B-D-Glucopyranosiduronic acid, 5-[2-hydroxy-3-[[2-(2-methoxyphenoxy)ethyl]amino]propoxy]-9H-carbazol-1-yl, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:17038 CAPLUS
DOCUMENT NUMBER: 114:17038
Identification of two major biliary metabolites of carvedilol in rats
AUTHOR(S): Pujimaki, M.: Hakusui, H.
CORPORATE SOURCE: Res. Inst., Daiichi Pharm. Co., Ltd., Tokyo, 134, Japan
SOURCE: Xenobiotica (1990), 20(10), 1025-34
CODEN: XENOBH; ISSN: 0049-8254
LANGUAGE: English
GI

DOCUMENT TYPE: LANGUAGE: GI

After sep. administration of R(+)-, S(-)-, and 14-C-labeled (i)-carvedilol [(i)-I) to rats at an oral dose of 10 mg/kg, the metabolic pattern in the bile was studied using (HPLC) with radioactivity and UV monitoring. Two major metabolites, present in the bile, accounted for 39 and 221, resp., of the dose. These metabolites were characterized as 1-hydroxycarvedilol O-glucuronide (II) and 8-hydroxycarvedilol O-glucuronide (III) and 8-hydroxycarvedilol N-glucuronide (III) and 8-hydroxycarvedilol N-glucuronide (III) and 8-hydroxycarvedilol N-glucuronide (III) resp., from fast atom bombardment-mass spectrometry, 1H-NMR and enzymic hydrolysis. Oral administration of R(+)-carvedilol

11

to highly selective excretion of II in bile, whereas S(-)-carvedilol resulted predominantly in excretion of III rather than II. 131087-98-4 [31087-99-5]
RL: BIOL (Biological study)
(as carvedilol metabolite, in bile)
131087-98-4 CAPLUS
B-D-Glucopyranosiduronic acid, 4-[2-hydroxy-3-[[2-(2-methoxyphenoxy)ethyl]amino]propoxy]-9H-carbazol-1-yl [9CI] (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) L3 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

131087-99-5 CAPLUS

B-D-Glucopyranosiduronic acid, 5-[2-hydroxy-3-[[2-(2-methoxyphenoxy)ethyl]amino]propoxy]-9H-carbazol-1-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1990:157993 CAPLUS 112:157993 TITLE: AUTHOR(S): Chakrabarti, Amit: Biswas, Gout

Photo-Fries rearrangements in N-sulfonylcarbazoles Chakrabarti, Amit; Biswas, Goutam K.; Chakraborty, D.

P.
Dep. Chem., Bose Inst., Calcutta, 700009, India
Tetrahedron (1989), 45(16), 5059-64
CODEN: TETRAB; ISSN: 0040-4020
JOURNAL
English
CASREACT 112:157993

CORPORATE SOURCE:

DOCUMENT TYPE:

LANGUAGE: OTHER SOURCE(S):

Photo-Fries rearrangement of N-sulfonyl carbazoles I (R = Ph, C6H4Me-4, Me) afforded the resp. 1- and 3-sulfonyl carbazoles in 29-55% yield. N-Benzoylcarbazole did not undergo similar rearrangement. 126230-30-6P 126230-31-7P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 126230-30-6 CAPLUS 9H-Carbazole, 1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

126230-31-7 CAPLUS
9H-Carbazole, 1-{(4-methylphenyl)sulfonyl}- (9CI) (CA INDEX NAME)

L3 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L3 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:449967 CAPLUS
111:49967 CAPLUS
1

X NYB N

GI

AB I (X = H, Me, F, Cl; R = e.g., CH2CH(OMe)2, (CH2)3NMe2, or CH2CH2OPh)
Were

prepared by the cyclization of monophenyl hydrazones of cyclohexane-1,2dione followed by treatment with corresponding amines and NaBH4
reduction The
antiviral activity of these compds. was studied against DNA-viruses
(herpes simplex) and RNA viruses both in culture cells and in mice. I (R
= PhCH2CH2 and X = Me) showed activity against both herpes and influenza
viruses in vivo. The activity was dependent on the structure of the
compds. e.g., I (R = CHMePh, X = Me: and R = CH2CH2Ph and X = H) Were
inactive.

1 118498-97-8P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antiviral activity of)

RN 118498-97-8 CAPLUS
CN 1H-Carbazol-1-amine, N-cyclohexyl-2,3,4,9-tetrahydro-6-methyl- (9CI) (CA
INDEX NAME)

L3 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L3 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:54362 CAPLUS

DOCUMENT NUMBER: 110:54362

AUTHOR(S): Synthesis and in vitro antituberculous activity of aikylaminotetrahydrocarboroles

AUTHOR(S): Filitis, L. N.; Akelaeva, T. V.; Amel'kin, O. Yu.;

Bokanov, A. I.; Ivanov, P. Yu.; Shvedov, V. I.

CORPORATE SOURCE: WHIKHI, Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1988), 22(10), 1217-22

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 110:54362

AB 1-Aminotetrahydrocarbazoles with various substituents at the exocyclic nitrogen atoms were synthesized and tested for their activity against Koch's bacilli, opportunistic mycobacteria, and saprophytes. All compds. were able to suppress the growth of mycobacteria in vitro but no therapeutic effect was found in mice with exptl. tuberculosis.

1 118498-97-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and tuberculostatic activity of, structure in relation to)

118498-97-8 CAPLUS

CN 118498-97-8 CAPLUS

L3 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:493909 CAPLUS
DOCUMENT NUMBER: 109:93909
The effect of heteroatomic substitutions on the band gap of polyacetylene and poly(p-phenylene)

derivatives AUTHOR (S): CORPORATE SOURCE:

Lee, Yong Sok; Kertesz, Miklos Dep. Chem., Georgetown Univ., Washington, DC, 20057, USA

SOURCE:

SOURCE: USA
SOURCE: Journal of Chemical Physics (1988), 88(4), 2609-17
CODEN: JCPSA6; ISSN: 0021-9606
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The electronic structures of poly(p-phenylene)(I), polyacetylene (II),

ABOUNDES:

English
ABO

The electronic structures of poly(p-phenylene)(I), polyacetylene (II),
and

their derivs. with small energy gaps were studied by the Hueckel and MNDO
crystal orbital methods. The effect of nuclear relaxation and heteroat.
substitution on the energy gaps [89] were taken into account by complete
geometry optimization using periodic boundary conditions as opposed to
earlier cluster-based calcus. Calcus. were done on: polypyrrole (III),
polythiophene (IV), poly(isothianaphthene) (V), poly(is,5'bithiophenemethenyl) (VI), and poly(5,5'-bipyrrolemethenyl (VII).
Energetics and band gaps for the 2 isomeric forms, the quinoid and
aromatic

structures of III and IV are discussed and critical compared with
previous

calcus. PMO theory is invoked to explain the narrower Eg for V, VI, and
VII relative to that of II. Calcus. for I derivs.,
(polybenzo[b]thiophene, polybenzo[b,f[thieno]3,4-c]thiophene, and
polybenzo[b]thiophene, polybenzo[b,f[thieno]3,4-c]thiophene, and
polybenzo[b]thiophene, polybenzo[b,f[thieno]3,4-c]thiophene, and
stabilize structures with desired small energy gaps are made. A
correlation of the Eg with heteroatom perturbation and geometrical
relaxation is given. The Eg is controlled not by aromatic vs. quinoid
contributions, but by the geometrical and heteroat. effects on the
frontier orbitals of the polymer.

IT 115980-71-7

RL: PRP (Properties)
(band gap of)

NN 15980-71-7 CAPLUS

CN Poly(4,8-dihydropyrrolo[2,3,4,5-def]carbazole-1,2,3:5,6,7-hexayl) (9CI)
(CA INDEX NAME)

L3 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:438899 CAPLUS
DOCUMENT NUMBER: 97:38899
TITLE: nitrenes. Part 10. The choice between carbazole and phenothiazine formation
AUTHOR(S): Hawkins, David G.; Meth-Cohn, Otto
CORPORATE SOURCE: Dep. Chem. Appl. Chem., Univ. Salford, Salford, M5
AUTHOR(S): Appl. Chem. (Property Company (1982) (A) Journal of Chemical Research, Synopses (1982), (4),

SOURCE:

CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE:

Journal English CASREACT 97:38899

LANGUAGE: OTHER SOURCE(S): GI

Thermal decomposition of the biphenyl I (R = N3) (II), prepared from 2,6-C12C6H3NO2 by sequential amination, phenylation, thiotolylation, and azidation, in 1,2,4-C13C6H3 for 3 h gave 81% carbazole II, whereas on hot PhOMe-sensitized photolysis 61% phenothiazine III was obtained. Deoxygenation of I (R = NO2) in 1,2,4-C13C6H3 under reflux for 24 h gave 17% II. The results are discussed in terms of a singlet nitrene origin for carbazole formation, with either singlet or triplet spin state giving the phenothiazine.
82342-01-6P
RL: RCT (Reactant): SDM (Symphotic arrange)

82342-01-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and desulfurization of) 82342-01-6 CAPLUS 9H-Carbazole, 1-{(4-methylphenyl}thio]- (9CI) (CA INDEX NAME)

ANSWER 29 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 30 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN L3 (Continued)

AUTHOR (S): B.;

L3 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:76484 CAPLUS
DOCUMENT NUMBER: 94:76484
TITLE: Metabolism of Carprofen, a nonsteroidal
antiinflammatory agent, in rats, dogs, and humans
AUTHOR(S): Rubio, F.; Seawall, S.; Pocelinko, R.; DeBarbieri,

Benz, W.: Berger, L.; Morgan, L.; Pao, J.; Williams, T. H.; Koechlin, B. Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
JOUrnal of Pharmaceutical Sciences (1980), 69(11), 1245-53
CODEN: JPMSAE; ISSN: 0022-3549
JOURNAL
English CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: GI

AB The metabolic disposition of 14C-labeled carprofen (I) [53716-49-7] was investigated in rats, dogs, and humans. In dogs and rats, the direct conjugation of I to form an ester glucuronide [76319-13-6] and oxidation to the C-7 (II) [76265-33-3] and the C-8 (III) [70359-64-7] phenols followed by their conjugation represent the major metabolic pathways. Small amts. of the α-hydroxy derivative [70359-62-5] also are formed by these species and are excreted free in the urine. In dogs, biliary secretion predominates, and 70% of an i.v. dose of I is excreted in the feces while 8-15% of the dose is excreted in the urine. In rats, fecal excretion due to biliary secretion varies from 60 to 75%, and urinary excretion accounts for 20-30% of an i.v. dose. In humans, direct conjugation of I represents the only significant pathway of metabolism Between 65 and 70% of the orally administered I was excreted as the ester glucuronide in the urine, and most of the remaining dose was estimated to be

secreted as this metabolite in the bile. Due to enterohepatic circulation, only a fraction of the biliary metabolite was recovered in the feces in humans. Less than 5% of the dose was excreted in human

e as free, intact I. In dogs and humans, plasma levels of I and of total radioactivity exhibit a multiphasic decline. In the human subjects studied, the terminal component declined with a 13-26-h half-life; the terminal half-life was .apprx.40 h in dogs. 75265-34-5.

76265-34-4
RL: BIOL (Biological study)
(as carprofen metabolite, species differences in)
76265-34-4 CAPLUS

ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) B-D-Glucopyranosiduronic acid, 7-(1-carboxyethyl)-3-chloro-9H-carboxol-1-yl (9C1) (CA INDEX NAME).

Absolute stereochemistry.

L3 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1953:6404 CAPLUS
DOCUMENT NUMBER: 47:6404
ORIGINAL REFERENCE NO: 47:1163e-i, 1164a-b
New syntheses of heterocyclic compounds. XVI. Ring
Closures involving loss of nitrous acid
BETG. S.: Closures involving loss of nitrous acid
BETG. S.: Petrow, V.
CORPORATE SOURCE: May 6 Baker, Ltd., Dagenham, UK
SOURCE: Journal of the Chemical Society (1952) 784-7
CODEN. JOSCAS JISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 46, 9564e. 2, 4,6-(02N)3C6H2C1 (I) (2.5 g.) and 2 g.
aminothiazole (II) in 30 ml. C6H6, refluxed 5 hrs., give 2.3 g. of a
complex, CHAMY2S.C6H2COR3C1, m. 80-110°. 2-Amino-4-methylthiazole
(10 g.) in 100 ml. boiling PhMe, treated with 11 g. I in 100 ml. PhMe and
refluxed 3 hrs., gives 10.2 g.
2,3-dihydro-4-methyl-2-picryliminothiazole,
crimson, m. 184-5°, ring closure could not be effected. The work
of Ochiał and Yanał (C.A. 35,743.6) was repeated (the condensation of I
with various pyrimidines) but the high yields for the cyclization could
not be reached. 6,8-Dinitro-1,9,11-triazafluorene (500 mg.) in 25 ml.
MeON, reduced (1 hr.) over 100 mg. Pt oxide, gives 200 mg.
6,8-diamino-1,9,11-triazafluorene, green, m. above 300°, 2-Me
derivative as the di-HGl salt, pale yellow, m. above 300°,
2-Amino-4-methylpyrimidine could not be condensed with
2,4-(OZN)2C6H3Br. 2,4,6-(OZN)3C6H2OMe (III) (2.5 g.) and 1 g.
2-aminopyrimidine (IV) in 15 ml. NeOH, refluxed 45 min., give 2.7 g. IV
picrate. III (2.4 g.), 0.95 g. IV, 3 g. AcONa, and 40 ml. MeON, refluxed
3 hrs., give 0.6 g. 2-(N-methylpicrylaminopyridine, yellow, m.
225-67; 1 g. II ylelds 700 mg. 2-(N-methylpicrylamino) phyridine, plane, blood red, m. 206-8°. 2-Picrylaminopyridine (IV) 10 film.
225-67; 1 g. II ylelds 700 mg. 2-(N-methylpicrylamino) phyridine, red, m. 242-6°, N-Methylation of
carbacole and PANH could not be effected. 2-Aminopyridine (V) (950 mg.)
and 2.6 g. 2,4,6-(OZN)3C6H2OBe (IV)2-Aminopyridine (V) (950 mg.)
and 2.6 g

229-31". 1,2,3,4-Tetrahydro-8-picrylaminocarbazole, red, m. 248"(decomposition), results in 13.5-g. yleld from 9.3 g. of the NH2 derivative; ring closure could not be effected by boiling quinoline,

derivative; ring closure could not be effected by boiling quinoline, t22 at 200°, hot alc. KOH, or by sublimation at 205-10°/0.03 mm.: PhOH-PhNO2 at 200° (0.5 hr.) gives a brown amorphous compound, C18H1404N4(7), m. above 300°. 1-Plcrylaminocarbazole, crimson, m. 274-5°, 801; PhNO2PhOH gives a red-brown amorphous compound, m. above 300°. 5-Chlorel-nembyl-4-nitroglyoxaline (8 g.), 5 g. o-H2NC6H4OH, 15 g. AcONa, a trace of KI, and 100 ml. EtOH, refluxed 24 hrs., give 6 g. 1-methyl-4-nitro-5-(o-hydroxyanilino)glyoxaline (VI), yellow, m. 222-4° (decomposition), red NaOH solution; 5 g. VI and 40 ml. EtZNH in 400 ml. EtOH, heated 16 hrs. at 120°, give 1.1 g. (from 1.5 l. AmOH) of blue needles (VII), C10H8ON3 (?) or C10H7ON3, m. above 310°; this may be the free-radical ayl (VIII) or the azhydrin (IX) structure, of which the latter is preferred. VII (4 g.) in 200 ml. entrated

HIZSO4, treated at 10-20° with 4 g. Zn, gives a pink compound [C10H7ON3 (?)], m. 250-5°, which is very rapidly oxidized to VII.

ANSWER 32 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN 854825-92-69, Carbazole, 1-(2,4,6-trinitroanilino)-(preparation of) 854825-92-6 CAPLUS (Continued)

854825-92-6 CAPLUS Carbazole, 1-(2,4,6-trinitroanilino)- (5CI) (CA INDEX NAME)

L3 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1931:6290 CAPLUS
DOCUMENT NUMBER: 25:6290
ORIGINAL REFERENCE NO: 25:716-i
INVENTOR(S): 1-Aminocarbazole
INVENTOR(S): Muth, Friedrich; Schmelzer, Albert
INVENTOR TYPE: PATENT
LANGUAGE: UNA. COUNT: PATENT INFORMATION:

1 Unavailable
PATENT INFORMATION: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DE 507797 19270314 DE

AB 1-Aminocarbazole and derivs. are prepared by first introducing the SO3H group into the carbazole mol., then introducing the NO2 group into the l-position, reducing it to the NH2 group, and finally removing the SO3H group if desired. Examples describe the preparation of sulfonic acid, 1-aminocarbazole-3,6,8-sulfonic acid, 1-aminocarbazole-3,6,8-sulfonic acid, 2-aminocarbazole-3,6,8-sulfonic acid, 2-aminocarbazole-3,6,8-sulfonic acid, 1-aminocarbazole-3,6,8-sulfonic acid,

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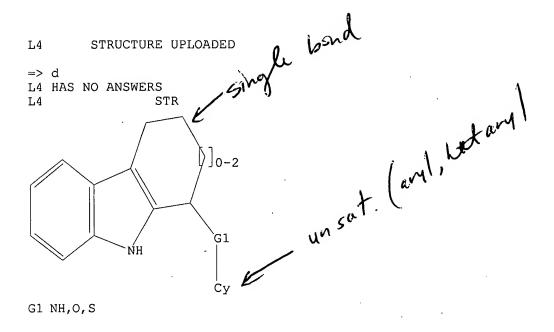
```
chain nodes :
16  17
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13
chain bonds :
13-16  16-17
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  7-10  8-9  8-13  10-11  11-12  12-13
exact/norm bonds :
5-7  6-9  7-8  7-10  8-9  8-13  11-12  13-16  16-17
exact bonds :
10-11  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
```

G1:NH,O,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 16:CLASS 17:Atom
Generic attributes:

17: Saturation

: Unsaturated



Structure attributes must be viewed using STN Express query preparation.

=> s 14 full sub=12 .
 REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 12:31:44 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 253 TO ITERATE

100.0% PROCESSED 253 ITERATIONS (3 INCOMPLETE) 98 ANSWERS

SEARCH TIME: 00.00.01

L5 98 SEA SUB=L2 SSS FUL L4

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH L6 10 L5

=> d ibib abs hitstr 1-10

TEPARTION of carbazoles and related compounds for treatment dengue fever, yellow fever, west nile virus, and inepatitis C virus infection. Gudmundsson, Kristjan Smithkline Mecham Corporation, USA PCT Int. Apl., 59pp. oppon: prXXD2 Patent English L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2006:1207231 CAPLUS 145:489114 TFTPART (on of carbacoles and treatment of dengue fever, years) INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English 1

20051114 GR, TR, TG, AM,

OTHER SOURCE(S):

MARPAT 145:489114

$$R_p$$
 N_n $XA(R^1)_q$ I

AB Title compds. [I; n = 0-2; X = NH, O, S, SO, SO2; R, Rl = halo, haloalkyl, alkenyl, alkenyl, cycloalkyl, aryl, aryloxy, arylamino, heterocyclyl, heterocyclyloxy, heterocyclylamino, cyano, NO2, N3, etc.;

q = 0-5; A = aryl, heteroaryl], were prepared for the treatment of infection

ttion due to flaviviruses, pestiviruses, and hepaciviruses. Thus, 6-chloro-N-phenyl-2,3,4,9-tetrahydro-lH-carbazol-l-amine (preparation outlined)

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-16-4 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

812649-17-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4-chlorophenyl)-2,3,4,9-tetrahydro-(CA INDEX NAME)

812649-18-6 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4-fluorophenyl)-2,3,4,9-tetrahydro-(CA INDEX NAME)

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) showed anti-HCV activity with ICSO = 5 nM.

812649-13-1P 812649-14-2P 812649-16-3P 812649-15-3P 812649-16-4P 812649-17-5P 812649-16-P 812649-19-7P 812649-21-7P 812649-21-1P 812649-22-2P 812649-23-3P 812649-21-1P 812649-25-5P 812649-23-3P 812649-21-P 812649-25-5P 812649-23-3P 812649-33-7P 812649-33-5P 812649-33-7P 812649-33-P 812

NAME)

812649-14-2 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

812649-15-3 CAPLUS . IH-Carbarol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-19-7 CAPLUS
1H-Carbazol-1-amine, 6-chloro-2, 3, 4, 9-tetrahydro-N-(4-methylphenyl)-CN (9CI) (CA INDEX NAME)

RN CN (9CI) 812649-20-0 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2, 3, 4, 9-tetrahydro-N-(4-methoxyphenyl)-(CA INDEX NAME)

812649-21-1 CAPLUS RN

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 1H-Carbazol-1-amine, 6-bromo-N-{4-chlorophenyl}-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-22-2 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(4-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-23-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyrimidinyl-,
monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued) 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

812649-27-7 CAPLUS 1H-Carbazol-1-amine, 6-chloro-N-(4,6-dimethyl-2-pyrimidinyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

812649-28-8 CAPLUS 1H-Carbazol-lamine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyridinyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

812649-24-4 CAPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

812649-25-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4,6-dimethoxy-2-pyrimidiny1)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-26-6 CAPLUS

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (9CI) (CA INDEX NAME) (Continued)

812649-30-2 CAPLUS 1H-Carbacol-l-maine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

812649-31-3 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methoxy-N-2-pyrimidinyl- (9CI)
(CA INDEX NAME)

RN 812649-32-4 CAPLUS
CN 1H-Carbazol-1-amine,
N-(4,6-dimethoxy-2-pyrimidinyl)-2,3,4,9-tetrahydro-6methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HC

RN 812649-33-5 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(4,6-dimethyl-2-pyrimidinyl)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

• HCl

RN 812649-34-6 CAPLUS
CN IH-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[5-(trifluoromethyl)-2-pyrimidinyl]- (9C1)
(CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-37-9 CAPLUS
CN IH-Carbazol-1-amine, N-2-benzothiazoly1-6-bromo-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

RN 812649-38-0 CAPLUS .

IN-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 812649-39-1 CAPLUS CN Cyclohept[b]indol-6-amine, 2-bromo-5,6,7,8,9,10-hexahydro-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

RN 812649-41-5 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyridinyl-,
monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-35-7 CAPLUS
CN | H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[5-(trifluoromethyl)-2-pyridinyl]- | 9Ct) | (CA | INDEX | NAME)

RN 812649-36-8 CAPLUS CN 3-Pyridinecarbonitrile, 6-((6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-y1)amino)- (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

• HCl

RN 812649-42-6 CAPLUS
CN 1H-Carbazole-6-carboxylic acid, 2,3,4,9-tetrahydro-1-(phenylamino)-, methyl ester (9CI) (CA INDEX NAME)

RN 812649-44-8 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 812649-45-9 CAPLUS CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continue

NHPh H

RN 812649-46-0 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(3-methoxyphenyl)(9CI)
(CA INDEX NAME)

MeO NH H

RN 812649-47-1 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-N-(3-fluorophenyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

NH H

RN 812649-48-2 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-1H-indol-5-yl- (9CI)
(CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

F NH H

RN 812649-52-8 CAPLUS
CN HH-Carbazol-1-amine, 6-bromo-N-(3,4-dichlorophenyl)-2,3,4,9-tetrahydro-(9C1) (CA INDEX NAME)

C1 NH H

RN 812649-53-9 CAPLUS
CN 1H-Carbazole, 6-bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 814255-17-9 CAPLUS
CN 3-Pyridinecarbonitrile, 6-[(2,3,4,9-tetrahydro-6-methyl-1H-carbazol-lyl)aminoj- (9C1) (CA INDEX NAME)

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

RN 812649-49-3 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(2-methoxyphenyl)(9CI)
(CA INDEX NAME)

MEO NH H

RN 812649-50-6 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(2-chlorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

C1 NH H

RN 812649-51-7 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-N-(2-fluoropheny1)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

L6 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1207230 CAPLUS
DOCUMENT NUMBER: 145:50040
TITLE: Treatment of prophylaxis of Flaviviridae viruses substituted 2,3,4 related compounds Gudmundsson, Kris Smithkline Beecka PCT Int. Appl, 7 CODEN: PIXXII Patent English using 9-tetrahydro-1H-carbazoles and INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: Corporation, USA DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2006121466 A2 20061116 D 2005-US41090 20051114

W: AE, AG, AL, AM, AT, AU, AZ, BEM, BB, BG, BR, BW, BY, BZ, CA, CH, CM, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, ET, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, AA, DM, MG, MK, NM, MM, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, VW, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, MR, NA, SD, SL, SZ, TZ, UG, ZM, ZW, NM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO: US 2004-629906P P 20041122

OTHER SOURCE(S):

MARPAT 145:500040

$$\mathbb{R}^{1} \xrightarrow{\mathbb{R}^{1}} \mathbb{R}^{\mathbb{N}^{1}} \xrightarrow{\mathbb{R}^{1}} \mathbb{R}^{\mathbb{N}^{2}} = \mathbb{R}^{\mathbb{N}^{2}} \times \mathbb{R}^{\mathbb{N}^{\mathbb{N}^{2}} \times \mathbb{R}^{\mathbb{N}^{2}} \times \mathbb{R}^{\mathbb{N}^{2}} \times \mathbb{R}^{\mathbb{N}^{2}} \times \mathbb{R}^{\mathbb{N}^{2}} \times \mathbb{R}^{\mathbb{N$$

The present invention relates to 2,3,4,9-tetrahydro-IH-carbazoles and related compds. (shown as I; variables defined below; e.g. N-benzyl-2,3,4,9-tetrahydrocarbazol-1-amine hydrochloride) that are

il in the treatment of viruses belonging to Flaviviridae, including flaviviruses, pestiviruses, and hepaciviruses. The invention includes compds. useful for the treatment or prophylaxis of dengue fever, yellow fever, West Nile virus, and HCV. For I: n = 0-2; R is H or alkyl; X is NR2. O, or S(0)m; each Rl = H, halogen, haloalkyl, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, -RlOcycloalkyl, Ay, -NHRlOAy, Het,

ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PREP (Preparation); USES (Uses)
(drug candidate; treatment or prophylaxis of Flaviviridae viruses L6

substituted 2,3,4,9-tetrahydro-1H-carbazoles and related compds.) 847988-06-1 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-, monohydrochloride, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HC1

847988-08-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride, (1S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HC1

using

847988-00-5P, N-(2,3-Dihydro-lH-inden-2-yl)-2,3,4,9-tetrahydro-lH-carbazol-1-amine monohydrochloride 847988-24-3P, N-(2,3-Dihydro-lH-inden-2-yl)-6-methyl-2,3,4,9-tetrahydro-lH-carbazol-1-amine monohydrochloride 847988-48-IP, 7-Bromo-N-(2,3-dihydro-lH-inden-2-yl)-2,3,4,9-tetrahydro-lH-carbazol-1-amine monohydrochloride RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; treatment or prophylaxis of Flaviviridae viruses

L6 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
-NHHet, -NHR10Het, -OR2, -OAy, - OHet, -R10OR2, -NR2R3, -NR2Ay, -R10NR2R3

R2R3,
et al.; Y is (un)substituted alkylene, cycloalkylene, alkenylene,
cycloalkenylene, or alkynylene; d = 0-1; Z is -R2, -CR2, -C(O)R2,
-C(O)2R2, -S(O)MR2, -C(O)NR2R3, -Het, or Ay, provided when d is 0, then Z
is not -Het or -Ay; each m = 0-2; each R10 = alkylene, cycloalkylene,
alkenylene, cycloalkenylene, and alkynylene; p = 0-4; each of R2 and R3 =
H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, -R10Cycloalkyl,
-R10CH, -R10(CR10)W, and -R10NRSR6; w = 1-10; each of R5 and R6 = alkyl,
cycloalkyl, alkenyl, cycloalkenyl, and alkynyl; Ay = (un)substituted

cycloalkyl, alkenyl, cycloalkenyl, and alkynyl; Ay = (un)substituted 5: or 6-membered heterocyclyl or heteroaryl group; addnl. details are given in the claims. Inhibition of MCV activity was measure for 3 examples of 1, e.g. 1C50 = 8 nM for (1R)-6-Bromc-N-(1R)-1-phenylethyl)-2, 3, 49-tetrahydro-1H-carbazol-1-amine hydrochloride. Although the methods of prepn. are not claimed, prepns. and/or characterization data for apprx.70 examples of 1 are included. For example. N-benzyl-2, 3, 4, 9-tetrahydrocarbazol-1-amine hydrochloride was prepd. (35 % yield) by addn. of sodium triacetoxyborohydride, acctic acid and benzylamine to a dichlorocethane soln. of 2, 3, 4, 9-tetrahydroc-1H-carbazol-1-one, which was prepd. in 2 steps from 4-chloroaniline, NaNO2 and 2-(hydroxymethylene)cyclohexanne in which the intermediate cyclohexane-1, 2-dione (4-chlorophenyl)hydrazone was cyclized. 847988-07-2, 6-Bromcon-(2, 3-dihydro-1H-inden-2-yl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine RL: PEP (Physical process) (Physical process) (Chromatog, resolution; treatment or prophylaxis of Flaviviridae ass

using substituted 2,3,4,9-tetrahydro-1H-carbazoles and related

compds.). 847988-07-2 CAPLUS
CN H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

847988-06-1P, (1R)-6-Bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride 847988-08-3P,

(1S) -6-Bromo-N-(2,3-dihydro-1H-inden-2-yll-2,3,4,9-tetrahydro-1H-carbazol-1-amine monohydrochloride RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) substituted 2,3,4,9-tetrahydro-1H-carbazoles and related compds.) 84798B-00-5 CAPLUS 1H-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME) L6

● RC1

847988-24-3 CAPLUS IH-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

HC1

847988-48-1 CAPLUS
IH-Carbazol-1-amine, 7-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:608619 CAPLUS
TITLE: 145:83213
Preparation of tetrahydrocarbazoles as active agents for inhibiting VEGF production by translational control
Lennox, William Joseph; Qi, Hongyan; Lee, Duck-Hyung; Choi, Soongyu; Moon, Young-Choon
PATENT ASSIGNEE(S): PTXCD2
PATENT TYPE: CODE: PTXCD2
DOCUMENT TYPE: PARGUAGE: English
PAMILU ACC. NUM. COUNT: BRITE TO THE PROPERTY OF THE PROPER DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.							DATE		- 1	APPL	I CAT		DATE					
						-												
WO	WO 2006065480					A2 20060622				WO 2	005-		20051123					
WO	2006		A3 20060803															
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,	
		ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	ΜA,	MD,	MG,	MK,	MN,	MW,	MX,	
		MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	
		SG,	SK,	SL,	SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UΑ,	UG,	US,	υz,	VC,	
		VN,	YU,	ZA,	ZM,	ZW												
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	5E,	SI,	SK,	TR,	BF,	ВJ,	
		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,	
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,	
		KG,	KZ,	MD,	RU,	TJ,	TM											
PRIORITY	IORITY APPLN. INFO.:								US 2004-629889P						P 20041123			
										US 2	004-	6337	38P		P 2	0041	206	
										110 2	004-	6302	03D		D 2	0041	227	

OTHER SOURCE(S):

MARPAT 145:83213

(Continued) ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

The present invention relates to methods, compds., and compns. for inhibiting angiogenesis. More particularly, the present invention ${\bf r}$

to methods, compds., and compns. for inhibiting VEGF production The

to methods, computes, and computes for inhibiting vibor production The computes I [X = NR9R10, N(alkyl)C(0) aryl, H, etc. (wherein R9, R10 = H, alkyl, aryl, etc.; or NR9R10 = mono- or bicyclic heterocyclic ringj; R1-R3

= H, OH, alkyl (wherein R1 may optionally form (un)substituted 5-11 membered mono- or bi-heterocyclic ring with X); n = 0-2; R4-R7 = H, OH, alkyl, etc.; W = N, O, S; R8 = H, alkyl, cycloalkyl, etc.; W in the provision) were prepared Thus, reacting amine II with 2,3-diformylthiophene followed by treating the intermediate lactam III with LAH in THF afforded IV which showed ECSO of <0.01 µM in an assay evaluating the ability of compda. I to modulate hypoxia-inducible endogenous VEGF expression.

IT 812649-13-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

812649-13-IP
RI: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of tetrahydrocarbaroles as active agents for inhibiting

production by translational control)
812649-13-1 CaPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA NAME)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN 812649-16-4P 812649-17-5P 812649-20-0P
812649-21-1P 812649-22-2P 812649-46-0P
812649-47-1P 812649-49-3P 812649-50-6P
812649-51-7P 812649-52-8P 812649-53-9P
812645-51-7P 812649-52-8P 812649-53-9P
812655-12-4P 814255-18-0P 833409-63-7P
893409-75-1P 893409-76-2P 893409-71-7P
893409-75-1P 893409-76-2P 893409-77-3P
893409-39-3P 893409-83-1P 893409-83-3P
893409-39-3P 893409-83-1P 893409-85-3P
893409-86-4P 893409-97-7P
893409-99-9P 893410-02-1P 893410-66-5P
893410-61-2P 893410-10-1P 893410-65-7P
893410-61-2P 893410-10-1P 893410-63-4P
893410-64-5P
R1: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (preparation of tetrahydrocarbazoles as active agents for inhibiting production by translational control)
812649-16-4 CAPLUS
HL-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-(9CI) (CA INDEX NAME) 812649-17-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4-chlorophenyl)-2,3,4,9-tetrahydro-

(CA INDEX NAME)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-20-0 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-{4-methoxyphenyl}-

812649-21-1 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(4-chlorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-22-2 CAPLUS 1H-Carbzool-1-maine, 6-bromo-N-(4-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-46-0 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(3-methoxyphenyl)-(CA INDEX NAME)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-47-1 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(3-fluorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

RN CN (9CI) 812649-49-3 CAPLUS 1H-Carbazol-1-amine, '6-bromo-2,3,4,9-tetrahydro-N-(2-methoxyphenyl)-(CA INDEX NAME)

812649-50-6 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(2-chlorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-51-7 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(2-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-52-8 CAPLUS
IH-Carbazol-1-amine, 6-bromo-N-(3,4-dichlorophenyl)-2,3,4,9-tetrahydro-(9C1) (CA INDEX NAME)

812649-53-9 CAPLUS 1H-Carbazole, 6-bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

814255-12-4 CAPLUS 1H-Carbazoi-1-maine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

N NH H N Br

RN 814255-18-0 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethyl)(SCI) (CA INDEX NAME)

NHPh H

RN 893409-63-7 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-{4-(trifluoromethyl)phenyl)- (9CI) (CA INDEX NAME)

CF3

RN 893409-67-1 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[4-(1-methylethyl)phenyl]- (9C1) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

RN 893409-76-2 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[4(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

F3C-0

RN 893409-77-3 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(3-chlorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

RN 893409-79-5 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(3,5-dimethylphenyl)-2,3,4,9-tetrahydro(9C1) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

NH H

RN 893409-69-3 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(4-phenoxyphenyl)(9CI)
(CA INDEX NAME)

oph NH H

RN 893409-71-7 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-phenyl- (9CI) (CA INDEX NAME)

NHPh H

RN 893409-75-1 CAPLUS 1H-Carbazol-1-amine, N-1,3-benzodioxol-5-yl-6-bromo-2,3,4,9-tetrahydro-(9C1) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Me Me

RN 893409-83-1 CAPLUS
CN 1H-Carbazol-1-amine, N-[1,1'-biphenyl]-4-yl-6-bromo-2,3,4,9-tetrahydro(9C1) (CA INDEX NAME)

Ph NH H

RN 893409-85-3 CAPLUS CN lH-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-pyrazinyl- (9CI) (CA INDEX NAME)

NH HH

RN 893409-86-4 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(2,3-difluorophenyl)-2,3,4,9-tetrahydro[9C1] (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

MH H H Br

RN 893409-87-5 CAPLUS
CN Cyclohept[b]indol-6-amine, 2-bromo-5,6,7,8,9,10-hexahydro-N-phenyl- (9CI)
(CA INDEX NAME)

NHPh H

RN 893409-88-6 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethoxy)(9C1) (CA INDEX NAME)

NHPh H N O-CF3

RN 893409-93-3 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-{4-(4-morpholinyl)phenyl}- (9CI) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 893409-99-9 CAPLUS
N14-Carbazol-1-amine, 7-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA
INDEX
NAME)

RN 693410-02-1 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-3-isoxazolyl- (9CI) (CA INDEX NAME)

RN 893410-06-5 CAPLUS
CN Acetamide, N-[4-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)amino]phenyl]- (9CI) (CA INDEX NAME)

RN 893410-08-7 CAPLUS
CN 1,4-Benzenediamine, N'-(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)-N,N-dimethyl- (9C1) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 893409-96-6 CAPLUS CN 1H-Carbazol-1-amine, 5-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

RN 893409-97-7 CAPLUS
CN Benzonitrile, 4-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)amino](9CI) (CA INDEX NAME)

L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 893410-10-1 CAPLUS
CN Benzeneethanol, 3-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-1-yl)amino](9CI) (CA INDEX NAME)

RN 893410-32-7 CAPLUS CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-1H-pyrrol-1-yl- (9CI) (CA INDEX NAME)

RN 893410-61-2 CAPLUS
CN 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

893410-62-3 CAPLUS
1H-Carbazol-1-amine, N-(4-chloropheny1)-2,3,4,9-tetrahydro-6-(trifluoromethy1)- {9CI} (CA INDEX NAME)

893410-63-4 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2006:128535 CAPLUS DOCUMENT NUMBER: 144:36946 Symphosic and Symphosic and

AUTHOR (S):

144:359346
Synthesis and SAR of substituted tetrahydrocarbazole derivatives as new NPY-1 antagonists
Di Fabio, Romano: Giovannini, Riccardo; Bertani,
Barbara; Borriello, Manuela; Bozzoli, Andrea; Donati,
Daniele; Falchi, Alessandro; Ghirlanda, Damiano;
Leslie, Colin P.; Pecunioso, Angelo; Rumboldt,
Giovanna; Spada, Simone
GlaxoSmithKline Medicines Research Centre, Verona,
37135, Italy
Bioorganic & Medicinal Chemistry Letters (2006),
16(6), 1749-1752
CODEN: BMCLES; ISSN: 0960-894X
Elsevier B.V.

CORPORATE SOURCE:

SOURCE:

Elsevier B.V. Journal

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE (S):

English CASREACT 144:369846

The SAR of a new series of tetrahydrocarbazole derivs. I [Rl = Me, 3-(l-piperidinyl)propyl, piperidin-4-ylmethyl, etc.; R2 = R, 4-morpholinyl, l-piperidinyl, 4-methyl-1-piperazinyl, etc.] is evaluated: the appropriate decoration of this template led to the identification of

new class of NPY-1 antagonists showing good in vitro potency and a promising in vivo pharmacokinetic profile in rat.
882033-76-3P 882033-77-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and SAR of amino(chlorophenoxy)tetrahydrocarbazolones as IT

NPY-1

antagonists)
882033-76-3 CAPLUS
1H-Carbazole, 1-(4-chlorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME) RN CN

ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN L6 (Continued)

893410-64-5 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-(trifluoromethyl)-N-(4-(trifluoromethyl)phenyl)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) L6

882033-77-4 CAPLUS
4H-Carbazol-4-one, 1-(4-chlorophenoxy)-1,2,3,9-tetrahydro- (9CI) (CA INDEX NAME) RN CN

THERE ARE 16 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: THIS

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:444285 CAPLUS
DOCUMENT NUMBER: 143:162008
Effects of fluorination on electronic and excited states of fused zinc oligoporphyrins
Yamaguchi, Yoich
SOURCE: KRI, Kyoto, 600-8813, Japan
Journal of Chemical Physics (2005), 122(18), 184702/1-184702/10
CODE: JCPSAG: ISSN: 0021-9606
American Institute of Physics
Journal of Chemical Physics
CODE: JCPSAG: ISSN: 0021-9606
American Institute of Physics

PUBLISHER:

American Institute of Physics

DOCUMENT TYPE:

Journal

ABD D. functional theory (DFT) has been applied to study the effect of fluorination on the electronic and excited states of fused zinc oligoporphyrins in the search for new functionalizing materials, such as n-type organic semiconductors. The excitation spectra of meso-tetrafluoro, and perfluoro zinc porphyrins, and their triply meso-meso-, B-B, and B-B-linked fluorinated zinc oligoporphyrins were systematically examined using the time-dependent DFT method. The effect of the perfluorination on the zinc porphyrin (ZnP) causes the maximum 1.12 eV and 1.42 eV drops for the highest occupied and LUMO (ROMO and LUMO, resp.) levels, resp. The electronic and excitation features of the fluorinated ZnPs are almost similar to the unfluorinated ones. However, the large antibonding contribution of the meso-fluorines disturbs the stabilization of the HOMO, resulting in a more effective reduction of both the HOMO-LUMO gaps and the lowest Q excitation energies with

the increasing number of porphyrins compared to the unfluorination and

other types of fluorinations. It is found that the infinite fused fluorinated ZnP tapes with narrow gap (-0.1 eV-0.2 eV) as predicted by using the periodic-DFT level are slightly inferior to the near-zero gap semimetallic unfluorinated ZnP tape as a conducting mol. wire. The combination of the condensation and the meso- and/or p-fluorination of ZnP can finely tune the LUMO level to the Fermi level of the electrodes for fabrication of n-type conducting materials. The fused fluoro-olioporphyrins may then become new n-type organic semiconductors, provided they are well crystallized with a high electron mobility, such as the recently synthesized perfluoropentacene.
859507-60-1

IT RL: PEP (Physical, engineering or chemical process); PRP (Properties);

(Physical process); PROC (Process)
(comparison; fluorination effect on electronic and excited states of fused zinc oligoporphyrins in relation of 59507-60-1 CAPLUS
Poly(5,15-difluoro-21H,23H-porphine-2,18,20:8,10,12-hexayl-kN21,kN22,kN23,kN24 (SP-4-1)-zinc complex) (9CI)
(CA INDEX NAME)

ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

REFERENCE COUNT: THIS

FORMAT

THERE ARE 61 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L6 ANSWER 6 OF 10
ACCESSION NUMBER:
DOCUMENT NUMBER:
171TLE:
INVENTOR(S):

PATENT ASSIGNEE(S)
SOURCE:
DOCUMENT TYPE:
PATENT ASSIGNEE(S)
DOCUMENT TYPE:
DOCUMENT TYPE:
PATENT ASPICE OF THE TYPE OF THE lensed indoles DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English KIND DATE APPLICATION NO.

A1 20050317 MO 2004-US17982

AM, AT, AU, AZ, BA, BB, BG, BR, BM, BY, CU, CZ, DE, DK, DM, DZ, EC, EZ, EG, ES, HR, HU, ID, IL, IN, IS, JP, KF, KG, KP, LIT, LU, LV, NA, MD, MG, MK, MN, MM, MX, FC, PH, PL, PT, RO, RU, SC, SO, SE, SG, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, KE, LS, MM, MZ, NA, SD, SL, SZ, CZ, UG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, PATENT NO. 0040607 CA, CM, GB GD, KZ, LC, NA, NI, SL, SY, ZM, 2W ZW, AM, DE, DK, RO, SE, MR, NE, disk 20040607 SE, MC, PT, SK, HR 20040607 20060224

OTHER SOURCE(S):

WO 2004-US17982

20030826 - SGM

The present invention relates to cycloalkyl[b] condensed indoles (shown I; variables defined below; e.g. 6-chloro-2,3,4,9-tetrahydro-1H-carbazol-1-

MARPAT 142:31668

847988-06-1P, (1R)-6-Bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-1H-carbazol-1-amine hydrochloride 847988-08-3P,

H-inden-2-y1)-2,3,4,9-tetrahydro-1H Page 59 Searched by Jason M. Nolan, Ph.D.

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) amine), including administration of pharmaceutically acceptable salts, solvates, and physiol. functional derivs. thereof, that are useful in the treatment of human papillomaviruses (HFVs), and also to the methods for the making and use of such compds. HFV inhibition values for 56 examples of I are reported. For I: n = 0-2: R is H or alkyl: X is NR2, O, or S(O)m; each R1 = H, halogen, haloalkyl, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, R10cycloalkyl, Ay, NHR10Ay, Het, NHHet, NHR10Het, ORZ, OAY, OHET, R10DGZ, NRZAY, NRZAY, R10C(O)RZ, C(O)RZ, COZRZ, R10COZRZ, C(O)NRZR3, C(O)NRZAY, lett. (Continued)

RIOC(O)RZ, CIONZ, COCKZ, KLOUCKZ, CLOUNKERS, CLOTPY, CLOTRICAS, Helt, Het, CLO(N)RIOLOR, CLOTRICAS, CLOTRICAS, CLOTRICAS, CLOTRICAS, CLOTRICAS, CLOTRICAS, CLOTRICAS, CLONINGRAS, RIOC(ONNINRARS, RIOC(ONNINRARS, S(O)ZNRZRS, S(O)ZNRZRS, RIOSOZNRCORZ, COSOZNRZRS, RIOSOZNRCORZ, S(O)MRZ, COMMINICORZ, ROSOZNRZRS, RIOSOZNRCORZ, S(O)MRZ, COMMINICORZ, CLOTRICAS, CLOTRICA

not claimed, .apprx.70 example prepns. are included. For example, 6-chloro-2,3,4,9-tetrahydro-1H-carbazol-1-amine was prepd. (52 %) from 6-chloro-2,3,4,9-tetrahydro-1H-carbazol-1-one, NH40Ac, and NaBH3CN in MeOH; the ketone was prepd. (88 %) by cyclization of ohexane-1,2-dione (4-chlorophenyl)hydrazone, which was prepd. (49 %) from the diazonium

of 4-chloroaniline and 2-(hydroxymethylene)cyclohexanone. 847988-07-2, 6-Bromo-N-(2,3-dihydro-lH-inden-2-yl)-2,3,4,9-tetrahydro-lH-carbazol-1-amine RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process) (chromatog. resolution; preparation of novel cycloalkyl[b] condensed les

for treating human papillomaviruses) 847988-07-2 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

1-amine hydrochloride
RL: PAC (Pharmacological activity): PUR (Purification or recovery); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(drug candidate; prepn. of novel cycloalkyl[b] condensed indoles for
treating human papillomaviruses)
847988-06-1 CAPLUS
1H-Carbarol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9tetrahydro-, monohydrochloride, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HC1

847988-08-3 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride, (15)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

847988-00-5P, N-(2,3-Dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-1H-carbazo1-1-amine hydrochloride 847988-24-3P, N-(2,3-Dihydro-1H-inden-2-y1)-6-methy1-2,3,4,9-tetrahydro-1H-carbazo1-1-

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) amine hydrochloride 847988-48-1P, 7-Bromo-N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine hydrochloride RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(drug candidate; prepn. of novel cycloalkyl[b] condensed indoles for treating human papillomaviruses)
847988-00-5 Captus
HH-Carbazol-1-amine, N-(2,3-dihydro-1H-inden-2-yl)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

847988-24-3 CAPLUS 1H-Carbazol-1-amine, N-{2,3-dihydro-1H-inden-2-y1}-2,3,4,9-tetrahydro-6-methy1-, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

847988-48-1 CAPLUS IH-Carbazol-1-amine, 7-bromo-N-(2,3-dihydro-1H-inden-2-y1)-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
142:74445
Preparation of tetrahydrocarbazole derivatives as human papillomaviruses inhibitors
Boggs, Sharon Davis; Gudmundsson, Kristjan S.;
Richardson, Leah D'Aurora; Sebahar, Paul Richard Smithkline Beecham Corporation, USA
SOURCE:
DOCUMENT TYPE:

CODEN: PIXXD2
Patent

DOCUMENT TYPE: Patent

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OTHER SOURCE(S):

WO 2004-US17660

MARPAT 142:74445

AB Title compds. represented by the formula I (wherein R, Rl = independently

20040607

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) halo(alkyl), (cyclo)alkenyl, (amino)aryl, etc.; X = NH, O or SOm; m = 1

n = 0-2; p, q = independently 0-5; A = (hetero)aryl; and pharmaceutically acceptable salts, solvates, and physiol. functional derivs. thereof] were prepd. as human papillomaviruses (HPV) inhibitors. For example, II was given in a multi-step synthesis starting from the reaction of 4-chloroaniline with 2-(hydroxymethylene)cyclohexanone. II showed inhibition of HPV 16 with IC50 values of 10 nM in W-12 cellular assay. Thus, I and their pharmaceutical compns, are useful for the treatment or prophylaxis of conditions or disorders due to HPV infection, such as

and cancers (no data).
B12649-13-1P, 6-Bromo-N-phenyl-2,3,4,9-tetrahydro-1H-carbazol-1-

B12649-13-1P, 6-Bromo-N-phenyl-2,3,4,9-tetrahydro-1H-carbazol-1-amine
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RCT (Reactant or reagent; USES (Uses) (preparation of tetrahydrocarbazole derivs. as human papilloma viruses inhibitors)
812649-13-1 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA

NAME)

812649-14-2P, 6-Bromo-N-phenyl-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine hydrochloride 812649-15-3P, 6-Chloro-N-phenyl-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-16-4P, 6-Chloro-N-(4-methoxyphenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-17-5P, 6-Chloro-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-18-6P, 6-Chloro-N-(4-fluorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-19-7P, 6-Chloro-N-(4-methylphenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-20-0P, 6-Bromo-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-21-1P, 6-Bromo-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-23-3P, 6-Bromo-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-23-3P, 6-Bromo-N-(4-chlorophenyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine hydrochloride 812649-24-4P, 6-Chloro-N-(pyrimidn-2-yyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-25-5P, 6-Chloro-N-(4, 6-dimethoxypyrimidin-2-yyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-25-5P, 6-Chloro-N-(4, 6-dimethoxypyrimidin-2-yyl)-2, 3, 4, 9-tetrahydro-1H-carbazol-1-amine 812649-26-6P

6-Chloro-N-(4-methylpyrimidin-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine 812649-27-7P, 6-Chloro-N-(4,6-dimethylpyrimidin-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine 812649-28-8P, 6-Bromo-N-(pyridin-2-yl)-2,3,4,9-tetrahydro-1H-carbazol-1-amine

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

812649-15-3 CÁPLUS 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)-(8CI) (CA INDEX NAME)

812649-17-5 CAPLUS
1H-Carbazol-1-amine, 6-chloro-N-(4-chlorophenyl)-2,3,4,9-tetrahydro-(CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) hydrochloride 812649-29-9P, 6-Bromo-N-(5-propylpyrimidin-2-yl)-2,3,4,9-tetrahydro-H-tearbarol-1-amine 812649-30-2P, 6-Methyl-N-(pyrimidin-2-yl)-2,3,4,9-tetrahydro-H-tearbarol-1-amine 812649-31-3P, 6-Methoxy-N-(pyrimidin-2-yl)-2,3,4,9-tetrahydro-H-carbarol-1-amine 812649-32-4P, N-(4,6-Dimethoxypyrimidin-2-yl)-6-methyl-2,3-M-y-tetrahydro-H-carbarol-1-amine 812649-32-4P, N-(4,6-Dimethoxypyrimidin-2-yl)-6-methyl-2,3-M-y-tetrahydro-H-carbarol-1-amine hydrochloride 812649-34-6F, 6-Bromo-N-(5-trifluoromethyl)pyrimidin-2-yl)-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-34-6F, 6-Bromo-N-(5-trifluoromethyl)pyrimidin-2-yl)-2,3,4,9-tetrahydro-H-carbarol-1-amine 812649-36-8P, 6-([6-Bromo-2,3,4,9-tetrahydro-H-carbarol-1-amine 812649-36-8P, 6-([6-Bromo-2,3,4,9-tetrahydro-H-carbarol-1-amine 812649-33-PP, N-(1,3-Bernothiazol-2-yl)-6-bromo-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-33-PP, N-(1,3-Bernothiazol-2-yl)-6-bromo-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-33-PP, 6-Methyl-N-(pyridin-2-yl)-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-42-6P, Methyl-1-amine 812649-41-PP, 6-Methyl-N-(pyridin-2-yl)-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-42-6P, Methyl-1-amine 812649-41-PP, 8-Methyl-N-(pyridin-2-yl)-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-42-6P, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-42-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-42-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-40-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-40-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-40-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-40-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-40-PP, N-Phenyl-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-52-8P, 6-Bromo-N-(2-methoxyphenyl)-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-52-8P, 6-Bromo-N-(3-methoxyphenyl)-2,3,4,9-tetrahydro-1H-carbarol-1-amine 812649-52-8P, 6-Bromo-N-(3-methoxyphenyl)-2,3,4,9-tetrahydro-1H-carbarol (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of tetrahydrocarbazole derivs. as human papilloma viruses inhibitors) 812649-14-2 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

812649-18-6 CAPLUS 1H-Carbazol-1-amine, 6-chloro-N-(4-fluorophenyl)-2,3,4,9-tetrahydro-(CA INDEX NAME)

812649-19-7 CAPLUS
1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methylphenyl)-(CA INDEX NAME)

RN 812649-20-0 CAPLUS

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(4-methoxyphenyl)(9C1)
(CA INDEX NAME)

RN 812649-21-1 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-N-(4-chlorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

RN 812649-22-2 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-N-(4-fluorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-23-3 CAPLUS CN 1H-Carbacol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-2-pyrimidinyl-, monohydrochloride (9CI) (CA INDEX NAME)

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RN 812649-24-4 CAPLUS
CN 1H-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI)
(CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-25-5 CAPLUS
CN IH-Carbazol-1-amine, 6-chloro-N-(4,6-dimethoxy-2-pyrimidinyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

RN 812649-26-6 CAPLUS
CN HH-Carbazol-1-amine, 6-chloro-2,3,4,9-tetrahydro-N-(4-methyl-2-pyrindinyl)- (9C1) (CA INDEX NAME)

RN 812649-27-7 CAPLUS
CN IH-Carbazol-1-amine, 6-chloro-N-(4,6-dimethyl-2-pyrimidinyl)-2,3,4,9-tetrahydro-(9CI) (CA INDEX NAME)

RN 812649-28-8 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2, 3, 4, 9-tetrahydro-N-2-pyridinyl-,
monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

RN 812649-29-9 CAPLUS CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(5-propyl-2-pyrimidinyl)-(9CI) (CA INDEX NAME)

RN 812649-30-2 CAPLUS CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

RN 812649-31-3 CAPLUS
CN 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methoxy-N-2-pyrimidinyl- (9CI)

(Continued)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (CA INDEX NAME) (Continued)

RN 812649-32-4 CAPLUS CN 1H-Carbazol-1-amine, N-(4,6-dimethoxy-2-pyrimidinyl)-2,3,4,9-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

812649-33-5 CAPLUS IH-Carbarol-1-amine, 6-bromo-N-{4,6-dimethyl-2-pyrimidinyl}-2,3,4,9-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

HC1

812649-34-6 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-[5-(trifluoromethyl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

812649-35-7 CAPLUS
1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-{5-(trifluoromethyl)-2-pyridinyl}- (9CI) (CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-36-8 CAPLUS
3-Byridinecarbonitrile, 6-[(6-bromo-2,3,4,9-tetrahydro-1H-carbazol-l-yllamino]- (9CI) (CA INDEX NAME)

812649-37-9 CAPLUS 1H-Carbarol-1-amine, N-2-benzothiazoly1-6-bromo-2, 3, 4, 9-tetrahydro- (9CI) (CA INDEX NAME)

812649-38-0 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

812649-39-1 CAPLUS Cyclohept[b]indol-6-amine, omo-5,6,7,8,9,10-hexahydro-N-2-pyrimidinyl-(9CI) (CA INDEX NAME)

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812649-41-5 CAPLUS 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-6-methyl-N-2-pyridinyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

812649-42-6 CAPLUS
1H-Carbazola-6-Carboxylic acid, 2,3,4,9-tetrahydro-1-(phenylamino)-, methyl ester (9C1) (CA INDEX NAME)

Searched by Jason M. Nolan, Ph.D.

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-43-7 CAPLUS
3-Pyridinecarbonitrile, 6-{(2,3,4,9-tetrahydro-6-methyl-1H-carbazol-1-yl}amino]-, monohydrochloride {9CI} (CA INDEX NAME)

812649-44-8 CAPLUS
1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl-6-(trifluoromethyl)-,
monohydrochloride (9C1) (CA INDEX NAME)

● HCl

812649-45-9 CAPLUS 1H-Carbazol-1-amine, 2,3,4,9-tetrahydro-N-phenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 812649-46-0 CAPLUS
CN 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(3-methoxyphenyl)-(9CI) (CA INDEX NAME)

812649-47-1 CAPLUS IH-Carbacol-Amine, 6-bromo-N-(3-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

812649-48-2 CAPLUS IH-Carbacol-l-maine, 6-bromo-2,3,4,9-tetrahydro-N-1H-indol-5-yl- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-49-3 CAPLUS 1H-Carbazol-1-amine, 6-bromo-2,3,4,9-tetrahydro-N-(2-methoxyphenyl)-(CA INDEX NAME)

812649-50-6 CAPLUS
1H-Carbazol-1-amine, 6-bromo-N-(2-chlorophenyl)-2,3,4,9-tetrahydro- (9CI)
(CA INDEX NAME)

812649-51-7 CAPLUS 1H-Carbazol-1-amine, 6-bromo-N-(2-fluorophenyl)-2,3,4,9-tetrahydro- (9CI) (CA INDEX NAME)

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

812649-52-8 CAPLUS IH-Carbazol-1-amine, 6-bromo-N-(3,4-dichlorophenyl)-2,3,4,9-tetrahydro-(9C1) (CA INDEX NAME)

812649-53-9 CAPLUS
1H-Carbazole, 6-bromo-1-(4-fluorophenoxy)-2,3,4,9-tetrahydro- (9CI) (CA
INDEX NAME)

REFERENCE COUNT:

FORMAT

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:726528 CAPLUS
DOCUMENT NUMBER: 139:371731
TITLE: Photophysical Properties of Directly Linked Linear
Porphyrin Arrays
AUTHOR(S): Kim, Dongho; Osuka, Atsuhiro
National Creative Research Initiatives Center for
Ultrafast Optical Characteristics Control and
Department of Chemiatry, Yonsei University, Scoul,
120-749, S. Korea

SOURCE: Journal of Physical Chemistry A (2003), 107(42),
8791-8816
CODEN: JPCAFH; ISSN: 1089-5639
American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: American Chemical Society
DOCUMENT TYPE: Tormal Properties of the Control and
electronics. From a viewpoint of operational requirements, the porphyrin
arrays should have the very regular pigment arrangements which allow a
facile light energy or charge flow along the arrays but do not result in
the alteration of individual properties of the constituent pigments
leading to formation of so-called energy or charge sink. In these
respects, the directly coupled (orthogonal and fused) porphyrin arrays
without any linkers are ideal, because the conformational heterogeneity
mainly arising from a dihedral angle distribution between the neighboring
porphyrin moieties should be minimized. In addition, the electronic
of the linker can be disregarded in design strategy of mol. photonic

porphyrin moieties should be minimized. In addition, the electronic of the linker can be disregarded in design strategy of mol. photonic devices, because the linker can also be considered as a transmission element in electronic communication. Considering these features, these types (orthogonal vs fused) of porphyrin arrays would be one of the most suitable synthetic mol. modules for the realization of mol. photonic and electronic devices. To unveil the functionalities of various porphyrin arrays, starting from the dihedral angle dependence on the photophys. properties of the porphyrin dimers, we have extended our knowledge to longer orthogonal and fused porphyrin arrays. Overall, the regularly arranged porphyrin arrays with ample electronic interactions will be promising in the applications such as mol. wires, sensors, optical nonlinear materials, and so on.

IT 486445-26-5
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP

(Physical process); PROC (Process)
(photophys. properties of directly linked linear porphyrin arrays)
486445-26-5 CAPLUS
Poly[[5,15-bis[4-{1,1-dimethyltridecyl]phenyl]-21H,23H-porphine2,20,18:8,10,12-hexayl-xN21,xN22,xN23,xN24] zinc
complex] (9CI) (CR INDEX NAME)

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

THERE ARE 121 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2002:870385 CAPLUS DOCUMENT NUMBER: 138:114936

138:114936
Photophysical properties of porphyrin tapes
Cho, Hyun Sun; Jeong, Dae Hong; Cho, Sung; Kim,
Dongho; Matsuzaki, Yoichi; Tanaka, Kazuyoshi; Tsuda,
Akihiko; Osuka, Atsuhiro
Center for Ultrafast Optical Characteristics Control
and Department of Chemistry, Yonsei University, TITLE: AUTHOR (S):

CORPORATE SOURCE:

Seoul.

120-749, S. Korea Journal of the American Chemical Society (2002), 124(49), 1642-14554 CODEN: JACSAT; ISSN: 0002-7863 American Chemical Society Journal SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: AB The novel

MENT TYPE: Journal JAGE: English English The novel fused Zn{II}porphyrin arrays (Tn, porphyrin tapes) in which the porphyrin macrocycles are triply linked at meso-meso, \$\textit{\textit{P}}\textit{\texti

absorption spectra of the porphyrin tapes show a systematic downshift to the IR region as the number of porphyrin pigments increases in the arrays.

The fused porphyrin arrays exhibit a rapid formation of the lowest

states (for T2, .apprx.500 fs) via fast internal conversion processes

photoexcitation at 400 nm (Soret bands), which is much faster than the internal conversion process of .apprx.1.2 ps observed for a monomeric Zn(II)

porphyrin. The relaxation dynamics of the lowest excited states of the porphyrin tapes were accelerated from .apprx.4.5 ps for the T2 dimer to .apprx.0.3 ps for the T6 hexamer as the number of porphyrin units

rases, being explained well by the energy gap law. The overall photophys. properties of the porphyrin tapes were observed to be in a sharp rast to contrast to

rast to those of the orthogonal porphyrin arrays. The PPP-SCI calculated charge-transfer probability indicates that the lowest excited state of

the porphyrin tapes (Tn) resembles a Wannier-type exciton closely, whereas

the lowest excited state of the directly linked porphyrin arrays can be considered as a Frenkel-type exciton. Conclusively, these unique photophys. properties of the porphyrin tapes have aroused much interest

in the fundamental photophysics of large flat organic mols. as well as in

the possible applications as elec. wires, IR sensors, and nonlinear optical materials. 486443-26-5 RE: PEP (Physical, engineering or chemical process); PRP (Properties); IT

PYP

(Physical process); PROC (Process)
(Photophys. properties of fused zinc porphyrin studied by
steady-stateand time-resolved spectroscopy and theor. MO calcns.)
RN 48645-26-5 CAPLUS

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continuer Poly[[5,15-bis[4-{1,1-dimethyltridecyllphenyl]-21H,23H-porphine-2,20,18:8,10,12-hexayl-kx21,kx22,kx23,kx24] zinc complex[(9CI) (CA INDEX NAME) (Continued)

PAGE 1-A

PAGE 1-B

THERE ARE 55 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:493909 CAPLUS
DOCUMENT NUMBER: 109:93909
The effect of heteroatomic substitutions on the band gap of polyacetylene and poly(p-phenylene)

derivatives AUTHOR(S): CORPORATE SOURCE:

derivatives
AUTHOR(S): Lee, Yong Sok; Kertesz, Miklos
CORPORATE SOURCE: Dep. Chem., Georgetown Univ., Washington, Dc, 20057,
USA
SOURCE: Journal of Chemical Physics (1988), 88(4), 2609-17
CODEN: JCPSA6; ISSN: 0021-9606

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The electronic structures of poly(p-phenylene)(I), polyacetylene (II), and

AB The electronic structures of poly(p-phenylene)(I), polyacetylene (II), and their derivs. with small energy gaps were studied by the Hueckel and NNDO crystal orbital methods. The effect of nuclear relaxation and heteroat. substitution on the energy gaps (Eg) were taken into account by complete geometry optimization using periodic boundary conditions as opposed to earlier cluster-based calcus. Calcus. were done on: polypyprole (III), polythiophene (IV), poly(isothianaphthene) (V), poly(5,5'-bithiophenemethenyl) (VI), and polyths,5'-bipyrolemethenyl (VII). Energetics and band gaps for the 2 isomeric forms, the quinoid and aromatic structures of III and IV are discussed and critical compared with previous calcus. PMO theory is invoked to explain the narrower Eg for V, VI, and VII relative to that of II. Calcus. for I derivs., (polybenzo[b]thiophene, polybenzo[b,f]thieno[3,4-c]thiophene, and polybenzo[b]thiophene, polybenzo[b,f]thieno[3,4-c]thiophene, and polybenzo[b]thiophene, polybenzo[b,f]thieno[3,4-c]thiophene, and correlation of the Eg with heteroatom perturbation and geometrical relaxation is given. The Eg is controlled not by aromatic vs. quinoid contributions, but by the geometrical and heteroat. effects on the frontier orbitals of the polymer.

IT 115980-71-7
RL: PRP (Properties) (band gap of)
RN 115980-71-7 CAPLUS
CN Poly(4,8-dihydropyrrolo[2,3,4,5-def]carbazole-1,2,3:5,6,7-hexayl) (9CI) (CA INDEX NAME)

L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)





10/560,013 02/26/2007

L3 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1931:6290 CAPLUS

DOCUMENT NUMBER: 25:6290
ORIGINAL REFERENCE NO.: 25:716h-i

TITLE: 1-Aminocarbazole

INVENTOR(S): Muth, Friedrich; Schmelzer, Albert

PATENT ASSIGNEE(S): I. G. Farbenindustrie AG

DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DE 507797 19270314 DE

AB 1-Aminocarbazole and derivs. are prepared by first introducing the SO3H group into the carbazole mol., then introducing the NO2 group into the 1-position, reducing it to the NH2 group, and finally removing the SO3H group if desired. Examples describe the preparation of 1-nitrocarbazole-3,6,8-sulfonic acid, 1-aminocarbazole-3,6,8-sulfonic acid, 1-aminocarbazole and 1-phenylaminocarbazole.

IT 859084-79-0P, Carbazole, 1-anilino-

RL: PREP (Preparation) (preparation of) 859084-79-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN